Technical documentation
WAQAD

Werkdocument RIKZ/OS-96.151X

Rijkswaterstaat
Ministerie van Infrastructuur en Milieu

Technical documentation WAQAD

The automatic calibration program

Version : 1.0, October 25, 1996
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Preface

The technical documentation of WAQAD was written as part of the project 'Extensions of WAQAD' (contract RKZ-232) commissioned by the National Institute for Coastal and Marine Management/RIKZ and carried out by SIMTECH, an independent engineering consultant specializing in civil and software engineering. It is a comprehensive compilation of the mathematical and technical aspects of WAQAD, the automatic calibration system. The following persons contributed text:

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This technical documentation is intended to meet the needs of persons wanting to know about:

- the mathematical (and theoretical) background of WAQAD,
- the WAQAD system itself and how the mathematical model is implemented.

Persons interested in using the WAQAD system in order to be able to calibrate models automatically are referred to the WAQAD User's Guide, [Brouwer, 1996b].

Persons starting to learn about the calibration process are advised to read some other books on this subject before reading this document. For example, the following documents are recommended:

- Inregelen van wiskundige modellen op basis van besturingstheorie, [Van den Boogaard, 1988]
- Data assimilation with altimetry techniques used in the Continental Shelf Model, [RIKZ, 1994]
- User's guide WAQAD, [Brouwer, 1996b]

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1. Introduction

It is generally recognized that mathematical models based on shallow water equations are useful for solving hydraulic problems in civil engineering. Such models are frequently used to calculate detailed flow patterns and to estimate water levels, so that water movement can be simulated. These computational flow models often contain empirical parameters which are not known very accurately.

The most crucial phase in the development of a hydrodynamic model is the calibration. Generally a model can be calibrated on the following parameters: bottom roughness, bottom topography and harmonic constituents in the boundary condition. All of these parameters are known only to a certain degree of accuracy and need to be optimally adjusted in the calibration process. The model builder is free to adapt these parameters within certain bounds. Observations are used for comparison with the model outcome and empirical parameters in the model are adjusted in order to improve the model's performance.

Flow models used to be calibrated fully manually by experts. This trial and error approach was very time consuming and laborious. In recent years advanced mathematical techniques in the field of optimal control theory have been successfully applied to model calibration. In a process generally called data assimilation, information derived from observations is combined with the model outcome, in order to improve the model's performance. The adjoint model developed by this process has become particularly popular. It is an inverse modelling technique in which misfits between computed and observed values are retranslated into adjustments of the model input. The more accurate the estimates of the parameters, the better the agreement between computed and observed water levels. The adjoint method enables models to be calibrated automatically and efficiently. Different parameters can be estimated simultaneously in an optimal way.

Using the adjoint method, an error function is introduced to quantify the misfit of the model outcome. This cost function is minimized by using an iterative algorithm: in each step of the iteration an improved vector of control variables is searched for, in a direction in the parameter space computed from the gradient of the cost function. The adjoint model computes this gradient vector efficiently. The adjoint method guarantees complete consistency with the dynamics.

RIKZ developed WAQAD, the automatic calibration program based on the adjoint method. The program calibrates two-dimensional shallow water flow models (WAQUA) by estimating depth, bottom friction, or boundary condition

parameters. WAQAD can also calibrate three-dimensional shallow water flow models (TRIWAQ) by estimating depth, bottom friction or vertical viscosity parameters.

WAQAD has been implemented in a SIMONA environment. One of the goals of the SIMONA project is to develop a generic framework in which it is easy to make connections between various (mathematical) modelling tools. The project also produces programming standards and documentation standards to make maintenance easier.

This documentation contains a complete description of the mathematical and technical aspects of WAQAD. Chapter 2 contains a general description of the adjoint method on which WAQAD is based. In chapter 3 the adjoint model for two-dimensional shallow water flow is described in detail: the adjoint model equations are derived, the adjoint solver as it is implemented in WAQAD is discussed and the derivation of the gradient is given. At the end of chapter 3 an overview of the remarks on WAQAD with respect to WAQUA is given. Chapter 4 focuses on the adjoint method for three-dimensional shallow water flow. Chapter 5 comprises a discussion of the potential, options and constraints of WAQAD in relation to identifiability and the use of the penalty, the use of weighting functions for parametrization, coupling harmonic constituents, analysis of the gradient in time and space, the use of current velocity measurements, friction formulations, finite difference calculations, and velocity and discharge boundaries. Finally, an overview of recommendations on WAQAD is given in chapter 6.

2. The adjoint method

The adjoint method is described in general in this chapter. It is outlined in section 2.1 and illustrated by means of the mathematical description in section 2.2

2.1. Introduction

The adjoint method is very important in off line data assimilation. It is used to make best estimates of uncertain parameters in a mathematical model. The mathematical theory for identifying parameters in distributed systems is based on [Chavent, 1980], and the methods for computing the shallow water equations are based on [Stelling, 1984]. The National Institute for Coastal and Marine Management/RIKZ has developed the technique of applying Chavent's method to models based on Stelling's method for conventional in-situ data, thereby combining advanced theory with important practical applications. The technique is outlined below.

The cost function J(p) provides an objective way of assigning preference to certain values of the parameters. This function is a measure of the model error. Usually the J(p) is chosen according to:

$$J(p) = \frac{1}{2} \sum_{m,n,k} \zeta^{k}_{m,n} \left[\zeta^{k}_{m,n}(p) - \hat{\zeta}^{k}_{m,n} \right]^2 \qquad (2.1)$$

with
- $\hat{\zeta}^{k}_{m,n}$ Observed water level at location m,n at time k
- p Vector of control variables
- $\zeta^{k}_{m,n}$ Model counterpart of observation

The summation in this quadratic criterion runs over all locations in the domain and over all time levels in the simulation period for which measurements are available. The control variables can be defined as additive or percentual correction factors for model parameters.

The set of parameters p is optimized in order to minimize the cost function J. The more accurate the estimates of the parameters, the better the agreement between computed and observed water levels, and the smaller the cost function. The best model performance can be achieved when the cost function reaches its minimum. To evaluate the cost function a model simulation has to be run for a given value of the parameters, to provide the computed water levels. The value of the cost function varies with the values chosen for the mathematical parameters. The cost function may be controlled by these uncertain parameters.

The gradient - i.e. the direction in which the parameters have to be adjusted so that the cost function will decrease - provides information crucial for searching efficiently for a more accurate estimate of the uncertain parameters. The minimum of the cost function can now be found iteratively. Ultimately

the optimal estimate of the uncertain parameters is determined. In other words: the mathematical model is calibrated.

The following steps are important in off-line data assimilation:

- Define the parameters in the mathematical model which have to be calibrated. In the case of a 2D simulation these may be: correction factors for the model values of the bottom friction, harmonic constituents in the boundary conditions, or depth. In the case of a 3D simulation they may be: correction factors for the model values of the bottom friction, the depth, or the vertical viscosity coefficient.
- Run a simulation with the original parameter values in the model and the correction factors initially set at zero. This gives a value for the initial cost function.
- Calculate the gradient of the cost function.
- Use a Quasi-Newtonian method in combination with a line minimization, to modify the correction factors which decrease the cost function.
- Stop if you are satisfied, or start again if you are not satisfied with the result.

It is well known that the minimum of a function is characterized by a zero gradient in all directions. The adjoint technique can be applied to determine the gradient of the criterion efficiently. Unlike other assimilation methods it has the advantage that the optimal estimate is consistent with the underlying physics of the model. The gradient can also be determined by another technique, called finite difference (see section 5.7). However, using this method the gradient cannot be calculated exactly. Therefore, the use of the finite difference method is restricted and not described in this section.

In the next section the adjoint method is illustrated by means of the mathematical description.

2.2. The mathematical description

When calibrating a shallow water flow model, one has to find the values for the uncertain parameters in the hydrodynamic model which minimize the cost function. As mentioned above, the lower the cost function, the better the agreement between computed and observed water levels. The water levels computed by the flow model are implicit functions of the uncertain parameters. The gradient of the criterion gives information about the direction (positive or negative) and the size (small or big) of the adjustments for each individual uncertain parameter. An adjoint method can be used to determine this gradient. The time needed to compute the gradient with the adjoint technique is more or less the same, regardless of the number of parameters, and is comparable with the computation time needed for one simulation run of the flow model (!).

The water level elevation ζ, and the velocity currents u and v flowing respectively east and north are the unknown variables in the mathematical model equations and are described by the laws of conservation of mass and by the conservation of momentum together with the model's boundary conditions. These descriptors are implicitly coupled in nonlinear partial differential equations. These shallow water equations contain some uncertain parameters, for example, bottom friction. If an additional correction factor is defined for the bottom roughness at a given location, the adjoint method can compute the derivative of the cost function with respect to this parameter only. This is comparable with a sensitivity analysis for this parameter. If more than one control parameter has to be estimated, the gradient becomes a vector.

The mathematical derivation of the adjoint equations and, concomitantly the determination of the gradient, will be outlined below. While searching for the optimal values, the physics of the model must not be violated. The constrained optimization problem is transformed into an unconstrained one by introducing Lagrange multipliers, [Bryson and Ho, 1975] and [Chavent, 1980]:

$$J(p)=\frac{1}{2}\sum_{m,n,k}\left[\zeta^{k}_{m,n}(p)-\hat{\zeta}^{k}_{m,n}\right]^2+\sum_{m,n,k}(\nu_\zeta)^{k+1}_{m,n}\,F_\zeta(\zeta,u,v,p)$$

$$+\sum_{m,n,k}(\nu_u)^{k+1}_{m,n}\,F_u(\zeta,u,v,p)+\sum_{m,n,k}(\nu_v)^{k+1}_{m,n}\,F_v(\zeta,u,v,p) \qquad (2.2)$$

The F_ζ functions state the conservation of mass; F_u and F_v state the conservation of momentum eastward and northward. These functions describe the physical processes of the

model, the propagation in time of the model state. They consists of finite difference methods for the continuous model equations, [Stelling, 1984].

Additional terms are appended to the cost function, each of which is the product of an undetermined multiplier and a model equation. Each model equation (for each discrete model variable at each grid point for every time step) must be associated with its own multiplier (the adjoint variable) and contribute one term. To simulate the flow the implicitly coupled model equations have to be solved for each grid point for each time level in the simulation period. Any value for an adjoint variable is allowed in (2.2), since the model state satisfies the model equations. More precisely, after the model simulation the corresponding model equation holds at each grid point for every time step:

$$F_\zeta(\bullet)=0\,,\ F_u(\bullet)=0\,,\ F_v(\bullet)=0$$

Note that there are exactly the same number of equations as there are unknown parameters.

To determine the gradient of the cost function expression (2.2) is differentiated with respect to one correction factor for an uncertain parameter. All discrete model variables are dependent on these uncertain parameters. The model state is a (difficult) implicit function of the correction factors. Therefore, the chain rule must be applied:

$$\frac{\partial J}{\partial p} = \sum_{m,n,k} \left[\ \zeta^k_{m,n}(p) - \hat{\zeta}^k_{m,n}\ \right] \frac{\partial \zeta^k_{m,n}}{\partial p}$$

$$+ \sum_{m,n,k} (\nu_\zeta)^{k+1}_{m,n} \left[\ \frac{\partial F_\zeta}{\partial \zeta}\frac{\partial \zeta}{\partial p} + \frac{\partial F_\zeta}{\partial u}\frac{\partial u}{\partial p} + \frac{\partial F_\zeta}{\partial v}\frac{\partial v}{\partial p} + \frac{\partial F_\zeta}{\partial p}\ \right] \qquad (2.3)$$

$$+ \sum_{m,n,k} (\nu_u)^{k+1}_{m,n} \left[\ \frac{\partial F_u}{\partial \zeta}\frac{\partial \zeta}{\partial p} + \frac{\partial F_u}{\partial u}\frac{\partial u}{\partial p} + \frac{\partial F_u}{\partial v}\frac{\partial v}{\partial p} + \frac{\partial F_u}{\partial p}\ \right]$$

$$+ \sum_{m,n,k} (\nu_v)^{k+1}_{m,n} \left[\ \frac{\partial F_v}{\partial \zeta}\frac{\partial \zeta}{\partial p} + \frac{\partial F_v}{\partial u}\frac{\partial u}{\partial p} + \frac{\partial F_v}{\partial v}\frac{\partial v}{\partial p} + \frac{\partial F_v}{\partial p}\ \right]$$

This expression still contains unknown terms for the gradient: namely all differentials of the water levels and the velocities with respect to an incremental change in the control parameter. For example, a local change in the bottom roughness also affects the tidal flow in other areas. In principle, changes in one parameter influence the water level

and the velocity current throughout the entire domain of the flow model. These influences are a priori unknown.

Looking more closely at the terms in this expression of the gradient (2.3), it can be seen that:

- The differentials of the model state at each location for every time step with respect to the parameter to be estimated are unknown. These terms are:

$$\frac{\partial \zeta}{\partial p}, \frac{\partial u}{\partial p}, \frac{\partial v}{\partial p}$$

- The differentials of the terms in the discretised model equations with respect to each individual model state at a certain point of time can be determined after simulating the tidal flow for the calibration period, in the case of a non-linear underlying forward model. These are:

$$\frac{\partial F_\zeta}{\partial \zeta}, \frac{\partial F_\zeta}{\partial u}, \frac{\partial F_\zeta}{\partial v}$$
$$\frac{\partial F_u}{\partial \zeta}, \frac{\partial F_u}{\partial u}, \frac{\partial F_u}{\partial v}$$
$$\frac{\partial F_v}{\partial \zeta}, \frac{\partial F_v}{\partial u}, \frac{\partial F_v}{\partial v}$$

- The differentials of the terms in the discretised model equations with respect to the control parameter can be determined after the simulation. These are:

$$\frac{\partial F_\zeta}{\partial p}, \frac{\partial F_u}{\partial p}, \frac{\partial F_v}{\partial p}$$

- The difference between the measurements and the computed water levels can be determined after the simulation. This term is:

$$\zeta(p) - \hat{\zeta}$$

So, known and unknown terms occur in this expression for the differential of the cost function with respect to the parameter. The adjoint variables ν_ζ, ν_u and ν_v are unrestricted. Any value is allowed. This gradient can be computed by the Chavent method. Rearranging the summation in (2.3) yields:

$$\frac{\partial J}{\partial p} = \sum_{m,n,k} \frac{\partial \zeta^k_{m,n}}{\partial p} \left[AF_\zeta(\nu_\zeta, \nu_u, \nu_v) + \left(\zeta^k_{m,n} - \hat{\zeta}^k_{m,n} \right) \right] + \sum_{m,n,k} \frac{\partial u^k_{m,n}}{\partial p} AF_u(\nu_\zeta, \nu_u, \nu_v) + \sum_{m,n,k} \frac{\partial v^k_{m,n}}{\partial p} AF_v(\nu_\zeta, \nu_u, \nu_v) + \sum_{m,n,k} \left[(\nu_\zeta)^k_{m,n} \frac{\partial F_\zeta}{\partial p} + (\nu_u)^k_{m,n} \frac{\partial F_u}{\partial p} + (\nu_v)^k_{m,n} \frac{\partial F_v}{\partial p} \right] \quad (2.4)$$

The AF functions describe the so-called adjoint equations. Every differential of a discrete model variable with respect to a control parameter is now associated with an adjoint equation (at each grid point for each time step). Similarly to the forward model, we can distinguish an 'inverse' continuity equation and 'inverse' momentum equations. If we select the Lagrange multipliers such that they satisfy the adjoint equations, the unknown terms in this expression for the gradient will be multiplied by zero. More precisely, the adjoint variables ν_ζ, ν_u and ν_v should be chosen such that at each grid point at every time step the corresponding adjoint equation holds:

$$AF_\zeta(\nu_\zeta, \nu_u, \nu_v) = \begin{cases} \hat{\zeta}^k_{m,n} - \zeta^k_{m,n} & \text{if measurement is available} \\ 0 & \text{if measurement is not available} \end{cases}$$

$$AF_u(\nu_\zeta, \nu_u, \nu_v) = 0$$

$$AF_v(\nu_\zeta, \nu_u, \nu_v) = 0$$

The unknown terms vanish, leaving a simple expression for the gradient of the criterion. The gradient for this selection of the adjoint variables can be computed:

$$\frac{\partial J}{\partial p} = \sum_{m,n,k} \left[(\nu_\zeta)^k_{m,n} \frac{\partial F_\zeta}{\partial p} + (\nu_u)^k_{m,n} \frac{\partial F_u}{\partial p} + (\nu_v)^k_{m,n} \frac{\partial F_v}{\partial p} \right]$$

The adjoint method is a so-called inverse model. The adjoint equations are solved going backwards in time, starting with a homogeneous 'initial' condition. Actually they describe the propagation reverse in time of the co-state. The adjoint system is activated by the disparity between the measurements and the computed model counterparts inside the system. Fortunately, the co-states in the interior are independent of the adjoint variables located at the boundaries: therefore, homogeneous adjoint boundary

conditions can be assumed. This property also holds for uncertain boundary conditions. Finally, the adjoint boundaries are determined by the adjoint solution for the inner points. Using the adjoint technique has several advantages:

- The adjoint equations are always linear even though there may be nonlinearities in the model equations. This is because the differential operator is linear.
- Computation is efficient, since the computational effort for the determination of the gradient of the criterion is not influenced by the number of control parameters. Integrating the adjoint equations backwards in time is more or less comparable with one forward model simulation.
- The inverse model is flexible in the sense that the number of parameters is easily changed. It is even possible to estimate different spatially varying correction factors for bottom roughness and harmonic constituents simultaneously. The only difference is the way the adjoint solution is combined with the original model output.
- With respect to the parameters to be estimated the Chavent method has two advantages over the conventional finite differences method for determining the gradient of the cost function: it computes the exact gradient and it is efficient.

There is only one disadvantage of using the adjoint technique:

- The computed water levels and velocities of each grid point at each time step during the calibration period have to be stored for use in the adjoint system. A shortage of disk space can be a serious problem, especially in the case of a 3D simulation. However, the technique of check-pointing can be used to overcome this problem. Using this technique, the calibration period is split into smaller periods that are calibrated separately and subsequently: when the first period is calibrated the data estimated in this period is used as restart data in the next period, which is then calibrated, and so on. For more information on this subject, see the WAQAD User's guide.

Once the gradient has been computed, the realm of minimising functions can be entered. As mentioned before, the gradient is a directional vector in the parameter space. Quasi-Newtonian formulae or conjugated gradient methods alter this direction to search for a better estimate. Nowadays experts generally agree that the BFGS (Broyden-Fletcher-Goldfarb-Shanno) updating formula is superior to others for medium-sized (<50) problems of parameter estimation. A line minimisation finds the values of the parameters along the search direction that have the lowest value of the cost function. With exact line minimisation a Quasi-Newtonian

method has second order convergence. For a thorough treatment of this topic the interested reader is referred to [Fletcher, 1987]. A short description of line minimisation is given below:

line search

When a new search direction is found, the stepsize that minimises the cost function J has to be determined. This search is performed in a forward or backward direction, depending on the value of the cost function J computed after the first estimation. When the value of the new computed J is larger than the original J, the optimum value is in-between and the search is performed backwards. Otherwise the search is performed forwards.

The forward search is performed with equal stepsizes defined by the parameter parcor, that is the initial parameter correction step size. The backward search is performed by reducing the previous stepsize to half its size.

Suppose that cost functions J_1, J_2, ..., J_n are computed during one iterative search process, the optimal step is then computed as follows:

- if ($J_2<J_1$) the search is performed forwards. The minimum value can be computed as soon as ($J_n>J_{n-1}$) with n>2 :

$$\text{step} = \tfrac{1}{2}\text{parcor}\left[\frac{3J_{n-2} - 4J_{n-1} + J_n}{J_{n-2} + J_n - 2J_{n-1}}\right]$$

3. The 2D adjoint model

This chapter describes the adjoint model for two-dimensional shallow water flow in detail. The adjoint model equations are derived in section 3.2. The adjoint solver as it is implemented in WAQAD is discussed in section 3.3. The derivation of the gradient is given in section 3.4. An overview of remarks on WAQAD with respect to WAQUA is shown in section 3.5.

A description of the three-dimensional adjoint model will be given in chapter 4.

3.1. Introduction

Flow models used to be calibrated fully manually by experts. This trial and error approach was very time consuming and laborious. In recent years advanced mathematical techniques in the field of optimal control theory have been successfully applied to model calibration. The adjoint model has become particularly popular.

In the early nineties RIKZ developed WAQAD, the automatic calibration program based on the adjoint method. The theory underlying WAQAD was derived by [Ten Brummelhuis, 1992] and implemented by J.R. Brouwer. This first version of WAQAD was designed in order to calibrate the two-dimensional shallow water flow model WAQUA. WAQUA models were calibrated automatically by estimation of depth parameters, bottom friction parameters or the wind stress coefficient (C_d). WAQAD was subsequently extended to calibrate WAQUA models by estimating the boundary conditions. Later, a second version of WAQAD was implemented in a SIMONA environment resulting from WAQUA-in-SIMONA. This version calibrates WAQUA-in-SIMONA models by estimating the depth, bottom friction and boundary parameters. However, estimation of the Cd coefficient was left out during this conversion. This second version is the current WAQAD version except for some extensions described by [Brouwer, 1995a] and [Brouwer, 1995b].

This chapter describes the 2D adjoint model as it is implemented in the current version of WAQAD: version 2.1, see the User's Guide WAQAD [Brouwer, 1996b] and the System Documentation of WAQAD [Brouwer, 1996a].

3.2. The adjoint model equations

This section focuses on the mathematical deduction of the adjoint model equations for depth averaged shallow water flow models. The method used here to derive the adjoint equations is the Chavent method outlined in chapter 2. The adjoint model equations are derived in section 3.2.1. Sections 3.2.2 to 3.2.4 describe advection, boundary conditions and dryfall, respectively.

3.2.1. Derivation of the adjoint model equations

The mathematical description of water flow consists of a system of coupled differential equations which are physically based on the conservation laws for mass and momentum. These shallow water equations are deduced from the well known Navier Stokes equations. Accordingly, the adjoint model is also mathematically described by differential equations.

Adjoint codes for mathematical models can be constructed in various ways. One way is to deduce the adjoint equations in continuous form from the continuous model equations and apply a finite difference scheme to obtain the discretized adjoint equations and the 'discretized' gradient. Chavent advises against using this approach. Another way is to apply adjoint model compilers which generate the adjoint code automatically, [Giering et al., 1995]. The great disadvantage of this is that the source code must be remoulded to the standards of the compiler. Rewriting the SIMONA environment to these standards (in combination with the complexity of the model) is quite a job. The best option is to employ the Chavent method on the discretized model equations to obtain the 'discrete' gradient i.e. the exact gradient of the discretized criterion.

To understand the mathematics of the adjoint model, it is necessary to understand the hydrodynamics of the forward model. The basic concepts of the latter reappear in the mathematical description of the inverse model. The depth-averaged shallow water equations are described in Cartesian coordinates by:

The u momentum equation, which describes the conservation of momentum in x direction:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} - fv + g\frac{\partial \zeta}{\partial x} + gu\frac{\sqrt{u^2 + v^2}}{C^2 H} - \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = F^{(y)} \tag{3.1}$$

The v momentum equation, which describes the conservation of momentum in y direction:

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial y} + u\frac{\partial v}{\partial x} + f\,u + g\frac{\partial \zeta}{\partial y} + g\,v\frac{\sqrt{u^2 + v^2}}{C^2 H} - \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) = F^{(y)} \tag{3.2}$$

The continuity equation, which describes the conservation of mass:

$$\frac{\partial \zeta}{\partial t} + \frac{\partial}{\partial x}(Hu) + \frac{\partial}{\partial y}(Hv) = 0 \tag{3.3}$$

in which:

u, v	=	Depth-averaged velocity components in the x and y directions
ζ	=	Water elevation above plane of reference
d	=	Water depth below plane of reference
H	=	Total water depth (d + ζ)
g	=	Acceleration due to gravity
C	=	Chezy coefficient for model bottom roughness
ν	=	Viscosity coefficient
f	=	Coriolis force
t	=	Time
$F^{(x)}$, $F^{(y)}$	=	External forces in the x and y directions

A two-stage time-splitting method is used to integrate the model equations for the two- dimensional shallow water flow model . The method is based on one used by [Stelling, 1984]. Because the model is used in a wide range of flow conditions, the discretization method used must be unconditionally stable and have at least second order accuracy. The discretization in

time is analogous to an ADI (Alternating Direction Implicit) method. Each stage describes the propagation of the model state in half a time step. In both stages the terms of the model equations are solved in a consistent way with at least second order accuracy in space. For example, if a term in the model equation is approximated implicitly in time in one stage, this term will be approximated explicitly in time in the other stage.

The spatially and temporally discretized equations for the two-dimensional hydrodynamic model are the starting point for deducing the corresponding adjoint equations, which are derived by following the next three steps:

- Determine the constraints in order to transform the constrained optimisation problem into an unconstrained one. These constraints are the non-linear discretisations of the shallow water equations described by (3.1)-(3.3).
- Derive the linearised equations. This is done in the following way: regard all WAQUA variables in the constraints as functions of the unknown model parameters. Then, differentiate the constraints to the model parameters.
- Rearrange the linearised equations by ordering the contributions of each multiplication factor. These contributions are the adjoint equations which must be solved.

The three steps are performed in the next part of this subsection. First, some remarks about the discretized equations:

- **Rectangular, spherical and curvilinear coordinates:** The discretisations of the model equations is dependent on the model grid used. In WAQAD there are three possibilities: the grid points can be given in rectangular co-ordinates, spherical co-ordinates or curvilinear co-ordinates. Rectangular and spherical co-ordinates are considered to be special cases of curvilinear co-ordinates. The following grid-dependent variables are used in the discretized equations:

  $\Delta\xi$ = grid distance in ξ direction
  $\Delta\eta$ = grid distance in η direction
  $K_{m,n}$ = distance between depth points in ξ direction
  $E_{m,n}$ = distance between depth points in η direction

  In the case of rectangular co-ordinates $\Delta\xi$ equals Δx and $\Delta\eta$ equals Δy, whereas $K_{m,n}$ and $E_{m,n}$ are both equal to 1.

  In the case of spherical co-ordinates the variables $K_{m,n}$ and $E_{m,n}$ are determined by:

$K_{m,n} = R \Delta\phi$
$E_{m,n} = R \cos \phi \Delta\lambda$

in which:

R = radius of the earth
ϕ,λ = grid angle in the northward and eastward directions

In the case of curvilinear coordinates the variables $K_{m,n}$ and $E_{m,n}$ are determined by:

$K_{m,n}$ = gvv = $\sqrt{g_{\xi\xi}}$, the WAQUA transformation coefficient in ξ direction

$E_{m,n}$ = guu = $\sqrt{g_{\eta\eta}}$, the WAQUA transformation coefficient in η direction

- **Time-dependent variables:**
  In the discretized equations state variables at different time levels are denoted as follows: the state variables at time level t+½Δt are denoted by a single apostrophe ('). The state variables at time level t+Δt are denoted by two apostrophes (''). If there is no apostrophe the state at time level t is meant.

- **Advection and viscosity:**
  The advection and viscosity terms have been ignored in the discretized equations given in this subsection. The horizontal advection terms of the discretized equations, which are taken into account in the 2D adjoint model, are described in subsection 3.2.2. The viscosity terms are not taken into account in the 2D adjoint model.

- **Changes arising from the implementation in WAQAD:**
  The discretized equations in this section were described in [Mouthaan, 1994]. However, some modifications regarding the formulation of bottom friction were made during the implementation of the equations in WAQAD, and these have been incorporated in this documentation: the equations described in this documentation are according to the WAQAD implementations.

Let us now perform the three steps.

Step 1: The WAQUA equations

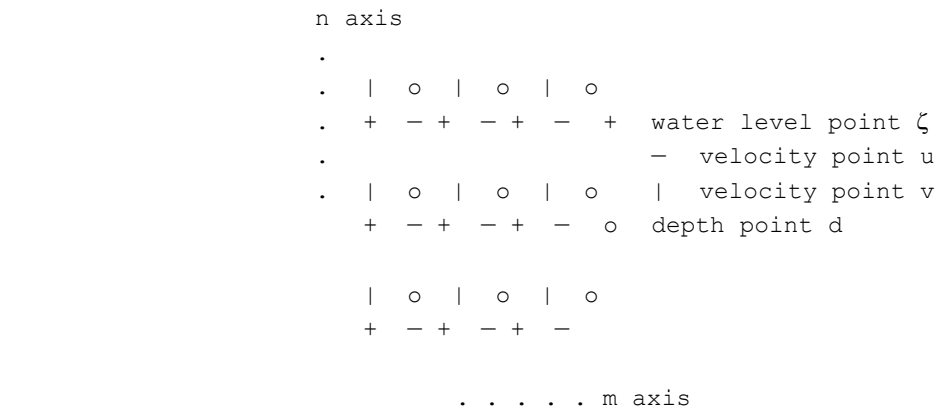


figure 3.1 The shaded points in the figure all have indices (m,n)

For an interior point in the field (see figure 3.1) not enclosed by any impeded geometry the discretized two-dimensional shallow water flow is described by:

- The v momentum equation in the first stage (from $t \rightarrow t+½\Delta t$). This is the first step of the ADI method in v direction. The WAQUA variables at time t are known. All v velocities at time $t+½\Delta t$ are calculated such that:

$$\frac{1}{½\,\Delta t}\left[\, v'_{m,n} - v_{m,n} \,\right] + \overline{f_{m,n}\, u_{m,n}}^{\xi\eta} + \frac{g}{E^{v}_{m,n}}\left[\, \frac{\zeta_{m,n+1} - \zeta_{m,n}}{\Delta\eta} \,\right] + \frac{g}{C_v^2}\,\frac{v_{m,n}\sqrt{\left(\overline{u_{m,n}}^{\xi\eta}\right)^2 + \left(v_{m,n}\right)^2}}{D^{v}_{m,n} + \overline{\zeta_{m,n}}^{\eta}} = 0 \qquad (3.4)$$

in which:

$v_{m,n}$	=	v velocity at time t
$v'_{m,n}$	=	v velocity at time $t+½\Delta t$
$D^{v}_{m,n}$	=	water depth at v velocity point: $½(d_{m-1,n}+d_{m,n})$
$E^{v}_{m,n}$	=	transformation coefficient E at v velocity point: $¼(E_{m-1,n}+E_{m,n}+E_{m,n+1}+E_{m-1,n+1})$
$f_{m,n}$	=	space-dependent Coriolis force
C_v	=	Chezy coefficient at v velocity point

and where the following terms are interpolated to v velocity points:

$$\bar{u}^{\xi\eta}_{m,n} = \tfrac{1}{4}[u_{m,n}+u_{m,n+1}+u_{m-1,n+1}+u_{m-1,n}]$$

$$\bar{\zeta}^{\eta}_{m,n} = \tfrac{1}{2}[\zeta_{m,n}+\zeta_{m,n+1}]$$

$$\overline{f_{m,n}u_{m,n}}^{\xi\eta} = \tfrac{1}{4}[f_{m,n}u_{m,n}+f_{m,n+1}u_{m,n+1}+f_{m-1,n+1}u_{m-1,n+1}+f_{m-1,n}u_{m-1,n}]$$

- The coupled equations in the first stage. This is the first step of the ADI method in u direction. The WAQUA variables at time t and the v velocities at time t+½Δt are known. All u velocities and water levels at time t+½Δt are calculated such that:

  the continuity equation is:

$$\frac{1}{\tfrac{1}{2}\Delta t}[\,\zeta'_{m,n} - \zeta_{m,n}\,] + \frac{1}{K^{\eta}_{m,n}E^{\xi}_{m,n}}\left\{\frac{1}{\Delta\xi}[\,(H^{u})'_{m,n}u'_{m,n}E_{m,n} - (H^{u})'_{m-1,n}u'_{m-1,n}E_{m-1,n}\,] + \frac{1}{\Delta\eta}[\,(H^{v})_{m,n}v_{m,n}K_{m,n} - (H^{v})_{m,n-1}v_{m,n-1}K_{m,n-1}\,]\right\} = 0 \qquad (3.5)$$

and the u momentum equation is:

$$\frac{1}{\frac{1}{2}\Delta t}[\,u'_{m,n} - u_{m,n}\,] - \overline{f_{m,n} v'_{m,n}}^{\eta\xi} + \frac{g}{K^{u}_{m,n}}\left[\frac{\zeta'_{m+1,n} - \zeta'_{m,n}}{\Delta\xi}\right] + \frac{g}{C_u^2}\frac{u'_{m,n}\sqrt{(u'_{m,n})^2 + (\overline{v'}^{\eta\xi}_{m,n})^2}}{D^{u}_{m,n} + \overline{\zeta'}^{\xi}_{m,n}} = 0 \qquad (3.6)$$

in which:

$(H^u)_{m,n}$ = total water depth at u velocity point: $\frac{1}{2}(\zeta_{m,n}+\zeta_{m+1,n}+d_{m,n}+d_{m,n-1})$

$(H^v)_{m,n}$ = total water depth at v velocity point: $\frac{1}{2}(\zeta_{m,n}+\zeta_{m,n+1}+d_{m-1,n}+d_{m,n})$

$K^{\eta}_{m,n}$ = transformation coefficient K at water level point: $\frac{1}{2}(K_{m,n-1}+K_{m,n})$

$E^{\xi}_{m,n}$ = transformation coefficient E at water level point: $\frac{1}{2}(E_{m-1,n}+E_{m,n})$

$K^{u}_{m,n}$ = transformation coefficient K at u velocity point: $\frac{1}{4}(K_{m,n-1}+K_{m+1,n-1}+K_{m+1,n}+K_{m,n})$

$D^{u}_{m,n}$ = water depth in u velocity point: $\frac{1}{2}(d_{m,n}+d_{m,n-1})$

C_u = chezy coefficient in u velocity point

and where the following terms are interpolated to u velocity points:

$\overline{v}^{\eta\xi}_{m,n}$ = $\frac{1}{4}[v_{m,n}+u_{m,n-1}+u_{m+1,n-1}+u_{m+1,n}]$

$\overline{\zeta}^{\xi}_{m,n}$ = $\frac{1}{2}[\zeta_{m,n}+\zeta_{m+1,n}]$

$\overline{f_{m,n} v_{m,n}}^{\eta\xi}$ = $\frac{1}{4}[f_{m,n}v_{m,n}+f_{m,n-1}v_{m,n-1}+f_{m+1,n-1}v_{m+1,n-1}+f_{m+1,n}v_{m+1,n}]$

- The u momentum equation at the second stage (from $t+½\Delta t \rightarrow t+\Delta t$). This is the second step of the ADI method in u direction. The WAQUA variables at time $t+½\Delta t$ are known. All u velocities at time $t+\Delta t$ are calculated such that:

$$\frac{1}{½\,\Delta t}[\,u''_{m,n} - u'_{m,n}\,] - \overline{f_{m,n}\,v'_{m,n}}^{\eta\xi}\,] + \frac{g}{K^u_{m,n}}\left[\frac{\zeta'_{m+1,n} - \zeta'_{m,n}}{\Delta\xi}\right] + \frac{g}{C_u^2}\frac{u'_{m,n}\sqrt{(u'_{m,n})^2 + (\overline{v'}^{\eta\xi}_{m,n})^2}}{D^u_{m,n} + \overline{\zeta'_{m,n}}^{\xi}} = 0 \qquad (3.7)$$

in which:

$u''_{m,n}$ = u velocity at time $t+\Delta t$

- The coupled equations in the second stage. This is the second step of the ADI method in v direction. The WAQUA variables at time $t+½\Delta t$ and the u velocities at time $t+\Delta t$ are known. All v velocities and water levels at time $t+\Delta t$ are calculated such that:

the continuity equation is:

$$\frac{1}{½\,\Delta t}[\,\zeta''_{m,n} - \zeta'_{m,n}\,] + \frac{1}{K^\eta_{m,n}E^\xi_{m,n}}\left\{\frac{1}{\Delta\xi}[\,(H^u)'_{m,n}u'_{m,n}E_{m,n} - (H^u)'_{m-1,n}u'_{m-1,n}E_{m-1,n}\,] + \frac{1}{\Delta\eta}[\,(H^v)''_{m,n}v''_{m,n}K_{m,n} - (H^v)''_{m,n-1}v''_{m,n-1}K_{m,n-1}\,]\right\} = 0 \qquad (3.8)$$

the v momentum equation is:

$$\frac{1}{½\,\Delta t}[\,v''_{m,n} - v'_{m,n}\,] + \overline{f_{m,n}\,u''_{m,n}}^{\xi\eta} + \frac{g}{E^v_{m,n}}\left[\frac{\zeta''_{m,n+1} - \zeta''_{m,n}}{\Delta\eta}\right] + \frac{g}{C_v^2}\frac{v''_{m,n}\sqrt{(\overline{u''}^{\xi\eta}_{m,n})^2 + (v''_{m,n})^2}}{D^v_{m,n} + \overline{\zeta''}^{\eta}_{m,n}} = 0 \qquad (3.9)$$

Step 2: The differentiated WAQUA equations

The WAQUA equations are differentiated to ζ, u and v applying the variational formalism:

- The differentiated v momentum equation at the first stage (from $t \rightarrow t+\frac{1}{2}\Delta t$), for $(\nu_v)'_{m,n}$ is:

$$\frac{1}{\frac{1}{2}\Delta t}[\,\Delta v'_{m,n} - \Delta v_{m,n}\,] + \overline{f_{m,n}\,\Delta u_{m,n}}^{\xi\eta} + \frac{g}{E^v_{m,n}}\left[\frac{\Delta\zeta_{m,n+1} - \Delta\zeta_{m,n}}{\Delta\eta}\right] + \overline{frvu_{m,n}\,\Delta u_{m,n}}^{\xi\eta} + frvv_{m,n}\,\Delta v_{m,n} + \overline{frvwl_{m,n}\,\Delta\zeta_{m,n}}^{\eta} \qquad (3.10)$$

in which:

frvu	=	contribution of bottom friction at v velocity point to the adjoint u momentum equation at time t
frvv	=	contribution of bottom friction at v velocity point to the adjoint v momentum equation at time t
frvwl	=	contribution of bottom friction at v velocity point to the adjoint continuity equation at time t

According to [Ten Brummelhuis, 1992] and [Brouwer, 1995b] the bottom friction contribution is given by:

$$\begin{aligned} frvu_{m,n} &= \frac{g}{C_v^2}\frac{\overline{u}^{\xi\eta}_{m,n}\,v_{m,n}}{(D^v_{m,n}+\overline{\zeta}^{\eta}_{m,n})\sqrt{(\overline{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}} \\ frvv_{m,n} &= \frac{g}{C_v^2}\frac{(\overline{u}^{\xi\eta}_{m,n})^2+2(v_{m,n})^2}{(D^v_{m,n}+\overline{\zeta}^{\eta}_{m,n})\sqrt{(\overline{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}} \\ frvwl_{m,n} &= -\frac{g}{C_v^2}\frac{v_{m,n}\sqrt{(\overline{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}}{(D^v_{m,n}+\overline{\zeta}^{\eta}_{m,n})^2} \end{aligned} \qquad (3.11)$$

Formula (3.11) describes the Chezy formulation. For further information on the friction formulation, see section 5.6 of this documentation.

Remark:
The overlined variables in equations (3.10) and (3.11) indicate that they are interpolated to v velocity points.

- The differentiated continuity equation in the first stage, for $(\nu_\zeta)'_{m,n}$:

$$\frac{1}{\frac{1}{2}\Delta t}[\Delta\zeta'_{m,n} - \Delta\zeta_{m,n}]$$
$$+\frac{1}{K^{\eta}_{m,n}E^{\xi}_{m,n}}\left\{\frac{1}{\Delta\xi}[(H^u)'_{m,n}E_{m,n}\Delta u'_{m,n}+\frac{1}{2}u'_{m,n}E_{m,n}(\Delta\zeta'_{m,n}+\Delta\zeta'_{m+1,n})]\right. \quad (3.12)$$
$$-\frac{1}{\Delta\xi}[(H^u)'_{m-1,n}E_{m-1,n}\Delta u'_{m-1,n}+\frac{1}{2}u'_{m-1,n}E_{m-1,n}(\Delta\zeta'_{m-1,n}+\Delta\zeta'_{m,n})]$$
$$+\frac{1}{\Delta\eta}[(H^v)_{m,n}K_{m,n}\Delta v_{m,n}+\frac{1}{2}v_{m,n}K_{m,n}(\Delta\zeta_{m,n}+\Delta\zeta_{m,n+1})]$$
$$\left.-\frac{1}{\Delta\eta}[(H^v)_{m,n-1}K_{m,n-1}\Delta v_{m,n-1}+\frac{1}{2}v_{m,n-1}K_{m,n-1}(\Delta\zeta_{m,n-1}+\Delta\zeta_{m,n})]\right\}$$

- The differentiated u momentum equation in the first stage, for $(\nu_u)'_{m,n}$ is:

$$\frac{1}{\frac{1}{2}\Delta t}[\Delta u'_{m,n} - \Delta u_{m,n}] - \overline{f_{m,n}\Delta v'_{m,n}}^{\eta\xi}$$
$$+\frac{g}{K^u_{m,n}}\left[\frac{\Delta\zeta'_{m+1,n}-\Delta\zeta'_{m,n}}{\Delta\xi}\right] \quad (3.13)$$
$$+ fruu'_{m,n}\Delta u'_{m,n} + \overline{fruv'_{m,n}\Delta v'_{m,n}}^{\eta\xi} + \overline{fruwl'_{m,n}\Delta\zeta'_{m,n}}^{\xi}$$

in which:

fruu'	=	contribution of bottom friction at u velocity point to the adjoint u momentum equation at time t+½Δt
fruv'	=	contribution of bottom friction at u velocity point to the adjoint v momentum equation at time t+½Δt
fruwl'	=	contribution of bottom friction at u velocity point to the adjoint continuity equation at time t+½Δt

The bottom friction contribution is given by:

$$
\begin{aligned}
fruu'_{m,n} &= \frac{g}{C_u^2}\frac{2(u'_{m,n})^2 + (\overline{v'}^{\eta\xi}_{m,n})^2}{(D^u_{m,n} + \overline{\zeta'}^{\xi'}_{m,n})\sqrt{(u'_{m,n})^2 + (\overline{v'}^{\eta\xi'}_{m,n})^2}} \\
fruv'_{m,n} &= \frac{g}{C_u^2}\frac{u'_{m,n}\,\overline{v'}^{\eta\xi}_{m,n}}{(D^u_{m,n} + \overline{\zeta'}^{\xi}_{m,n})\sqrt{(u'_{m,n})^2 + (\overline{v'}^{\eta\xi}_{m,n})^2}} \qquad (3.14) \\
fruwl'_{m,n} &= -\frac{g}{C_u^2}\frac{u'_{m,n}\sqrt{(u'_{m,n})^2 + (\overline{v'}^{\eta\xi}_{m,n})^2}}{(D^u_{m,n} + \overline{\zeta'}^{\xi}_{m,n})^2}
\end{aligned}
$$

Formula (3.14) describes the Chezy formulation. For further information on the friction formulation, see section 5.6 of this documentation.

Remark:
The overlined variables in equations (3.13) and (3.14) indicate that they are interpolated to u velocity points. This notation will be used in this documentation from now on.

- The differentiated u momentum equation in the second stage
(from t+½Δt → t+Δt), for $(\nu_u)''_{m,n}$ is:

$$
\begin{aligned}
&\frac{1}{\frac{1}{2}\Delta t}[\,\Delta u''_{m,n} - \Delta u'_{m,n}\,] - \overline{f_{m,n}\,\Delta v'_{m,n}}^{\eta\xi} \\
&\qquad + \frac{g}{K^u_{m,n}}\left[\frac{\Delta\zeta'_{m+1,n} - \Delta\zeta'_{m,n}}{\Delta\xi}\right] \qquad (3.15) \\
&+ fruu'_{m,n}\,\Delta u'_{m,n} + \overline{fruv'_{m,n}\,\Delta v'_{m,n}}^{\eta\xi} + \overline{fruwl'_{m,n}\,\Delta\zeta'_{m,n}}^{\xi}
\end{aligned}
$$

with fruu', fruv' and fruwl' given by (3.14).

- The differentiated continuity equation in the second stage, for $(\nu_\zeta)''_{m,n}$ is:

$$\begin{aligned}
&\frac{1}{\frac{1}{2}\Delta t}\left[\,\Delta\zeta''_{m,n} - \Delta\zeta'_{m,n}\,\right] \\
&+\frac{1}{K^{\eta}_{m,n}E^{\xi}_{m,n}}\left\{\frac{1}{\Delta\xi}\left[\,(H^{u})'_{m,n}E_{m,n}\Delta u'_{m,n}+\frac{1}{2}u'_{m,n}E_{m,n}\left(\Delta\zeta'_{m,n}+\Delta\zeta'_{m+1,n}\right)\right]\right. \\
&-\frac{1}{\Delta\xi}\left[\,(H^{u})'_{m-1,n}E_{m-1,n}\Delta u'_{m-1,n}+\frac{1}{2}u'_{m-1,n}E_{m-1,n}\left(\Delta\zeta'_{m-1,n}+\Delta\zeta'_{m,n}\right)\right] \\
&+\frac{1}{\Delta\eta}\left[\,(H^{v})''_{m,n}K_{m,n}\Delta v''_{m,n}+\frac{1}{2}v''_{m,n}K_{m,n}\left(\Delta\zeta''_{m,n}+\Delta\zeta''_{m,n+1}\right)\right] \\
&\left.-\frac{1}{\Delta\eta}\left[\,(H^{v})''_{m,n-1}K_{m,n-1}\Delta v''_{m,n-1}+\frac{1}{2}v''_{m,n-1}K_{m,n-1}\left(\Delta\zeta''_{m,n-1}+\Delta\zeta''_{m,n}\right)\right]\right\}
\end{aligned} \tag{3.16}$$

The differentiated v momentum equation in the second stage, for $(\nu_v)''_{m,n}$ is:

$$\begin{aligned}
&\frac{1}{\frac{1}{2}\Delta t}\left[\,\Delta v''_{m,n} - \Delta v'_{m,n}\,\right] + \overline{f_{m,n}\Delta u''_{m,n}}^{\xi\eta} \\
&+\frac{g}{E^{v}_{m,n}}\left[\,\frac{\Delta\zeta''_{m,n+1}-\Delta\zeta''_{m,n}}{\Delta\eta}\,\right] \\
&+\overline{frv\,u''_{m,n}\,\Delta u''_{m,n}}^{\xi\eta} + frv\,v''_{m,n}\,\Delta v''_{m,n} + \overline{frvw\,l''_{m,n}\,\Delta\zeta''_{m,n}}^{\eta}
\end{aligned} \tag{3.17}$$

with frvu'', frvv'' and frvwl'' given by (3.11), but at time t+Δt instead of time t.

Step 3: The adjoint equations

- The coupled adjoint equations in the first stage (from t+Δt $\rightarrow$ t+½Δt). The WAQAD variables at time t+Δt are known. All adjoint u velocities and adjoint water levels at time t+½Δt are calculated such that:

the adjoint continuity equation is:

$$\frac{1}{\frac{1}{2}\Delta t}\left[(\nu_\zeta)'_{m,n} - (\nu_\zeta)''_{m,n} \right]$$
$$+ \frac{g}{\Delta\xi}\left[\frac{(\nu_u)'_{m-1,n} + (\nu_u)''_{m-1,n}}{K^u_{m-1,n}} - \frac{(\nu_u)'_{m,n} + (\nu_u)''_{m,n}}{K^u_{m,n}} \right]$$
$$+ \frac{\frac{1}{2}u'_{m,n} E_{m,n}}{\Delta\xi}\left[\frac{(\nu_\zeta)'_{m,n} + (\nu_\zeta)''_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} - \frac{(\nu_\zeta)'_{m+1,n} + (\nu_\zeta)''_{m+1,n}}{K^\eta_{m+1,n} E^\xi_{m+1,n}} \right] \qquad (3.18)$$
$$+ \frac{\frac{1}{2}u'_{m-1,n} E_{m-1,n}}{\Delta\xi}\left[\frac{(\nu_\zeta)'_{m-1,n} + (\nu_\zeta)''_{m-1,n}}{K^\eta_{m-1,n} E^\xi_{m-1,n}} - \frac{(\nu_\zeta)'_{m,n} + (\nu_\zeta)''_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} \right]$$

$$+ \overline{fruw\, l'_{m-1,n}\left[(\nu_u)'_{m-1,n} + (\nu_u)''_{m-1,n} \right]}^{\xi} = 0$$

the adjoint u momentum equation is:

$$\frac{1}{\frac{1}{2}\Delta t}\left[(\nu_u)'_{m,n} - (\nu_u)''_{m,n} \right]$$
$$+ \frac{(H^u)'_{m,n} E_{m,n}}{\Delta\xi}\left[\frac{(\nu_\zeta)'_{m,n} + (\nu_\zeta)''_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} - \frac{(\nu_\zeta)'_{m+1,n} + (\nu_\zeta)''_{m+1,n}}{K^\eta_{m+1,n} E^\xi_{m+1,n}} \right] \qquad (3.19)$$

$$+ fruu'_{m,n}\left[(\nu_u)'_{m,n} + (\nu_u)''_{m,n} \right] = 0$$

- The adjoint v momentum equation in the first stage. The WAQAD variables at time t+Δt and the adjoint u velocities and adjoint water levels at time t+½Δt are known. All adjoint v velocities at time t+½Δt are calculated such that:

$$\frac{1}{\frac{1}{2}\Delta t}\left[(\nu_v)'_{m,n} - (\nu_v)''_{m,n} \right] - \overline{\left[f_{m,n} + fruv'_{m,n} \right]\left[(\nu_u)'_{m,n} + (\nu_u)''_{m,n} \right]}^{\xi\eta} = 0 \qquad (3.20)$$

- The coupled equations in the second stage (from t+½Δt $\rightarrow$ t). The WAQAD variables at time t+½Δt are known. All adjoint v velocities and adjoint water levels at time t are calculated such that:

  the adjoint continuity equation is:

$$\frac{1}{\frac{1}{2}\Delta t}\left[(\nu_\zeta)_{m,n} - (\nu_\zeta)'_{m,n} \right]$$

$$+ \frac{g}{\Delta\eta}\left[\frac{(\nu_v)_{m,n-1} + (\nu_v)'_{m,n-1}}{E^v_{m,n-1}} - \frac{(\nu_v)_{m,n} + (\nu_v)'_{m,n}}{E^v_{m,n}} \right]$$

$$+ \frac{\frac{1}{2} v_{m,n} K_{m,n}}{\Delta\eta}\left[\frac{(\nu_\zeta)_{m,n} + (\nu_\zeta)'_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} - \frac{(\nu_\zeta)_{m,n+1} + (\nu_\zeta)'_{m,n+1}}{K^\eta_{m,n+1} E^\xi_{m,n+1}} \right] \qquad (3.21)$$

$$+ \frac{\frac{1}{2} v_{m,n-1} K_{m,n-1}}{\Delta\eta}\left[\frac{(\nu_\zeta)_{m,n-1} + (\nu_\zeta)'_{m,n-1}}{K^\eta_{m,n-1} E^\xi_{m,n-1}} - \frac{(\nu_\zeta)_{m,n} + (\nu_\zeta)'_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} \right]$$

$$+ \overline{frvwl_{m,n-1}\left[(\nu_v)_{m,n-1} + (\nu_v)'_{m,n-1} \right]}^{\eta} = 0$$

the adjoint v momentum equation is:

$$\frac{1}{\frac{1}{2}\Delta t}\left[(\nu_v)_{m,n} - (\nu_v)'_{m,n} \right]$$

$$+ \frac{(H^v)_{m,n} K_{m,n}}{\Delta\eta}\left[\frac{(\nu_\zeta)_{m,n} + (\nu_\zeta)'_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} - \frac{(\nu_\zeta)_{m,n+1} + (\nu_\zeta)'_{m,n+1}}{K^\eta_{m,n+1} E^\xi_{m,n+1}} \right] \qquad (3.22)$$

$$+ frvv_{m,n}\left[(\nu_v)_{m,n} + (\nu_v)'_{m,n} \right] = 0$$

- The adjoint u momentum equation in the second stage. The WAQAD variables at time t+Δt and the adjoint v velocities at time t+½Δt are known. All adjoint u velocities at time t are calculated such that:

$$\frac{1}{\frac{1}{2}\Delta t}\left[(\nu_u)_{m,n} - (\nu_u)'_{m,n} \right] + \overline{\left[f_{m,n} + frvu_{m,n} \right]\left[(\nu_v)_{m,n} + (\nu_v)'_{m,n} \right]}^{\eta\xi} \qquad (3.23)$$

Remarks:

- The adjoint model equations are solved backwards in time. The initial condition for solving the equations is equal to zero.

- The adjoint model is activated by the misfits between the observed data and the corresponding model values. Residuals of observed and computed water levels affect the adjoint continuity equation. If a water level measurement has been recorded at a full time level, the residual has to be added to the right-hand side of the

corresponding adjoint continuity equation (3.21) at the second stage.

- Homogeneous boundary conditions are assumed for calculation of the adjoint state variables in the interior model field. Only if uncertain parameters of the WAQUA boundary conditions are estimated do the corresponding adjoint variables at the boundary have to be calculated afterwards. This is described in subsection 3.2.3.

3.2.2. Advection

3.2.2.1. Introduction

Advective terms can play an important role in modelling the flow in estuaries, [Stelling, 1984]. Such terms occur only in the conservation of momentum. These terms are uu_x and vu_y in the u momentum equation and vv_y and uv_x in the v momentum equation. In the first stage in WAQUA the v momentum equation is solved first and then the continuity equation and the u momentum equation are solved together. In the second stage in WAQUA the u momentum equation is solved first and then the continuity equation and the v momentum equation are solved together.

In subsection 3.2.2.2 the structure of the solution method of the discretized WAQUA equations with advection terms is described. For simplicity the external forces are set equal to zero. In order to obtain a unique solution to the discretized equations, a set of boundary conditions has to be prescribed. The boundary treatment is ignored throughout this section. See appendix A for information on boundary conditions and dryfall with advection.
Subsection 3.2.2.3 gives a derivation of the adjoint advection terms. In that subsection and subsection 3.2.2.2 the advective terms are described using rectangular coordinates. This is followed, in subsection 3.2.2.4, by an overview of the differences between rectangular, curvilinear and spherical coordinates.

3.2.2.2. Advective terms in WAQUA

In this subsection the computation procedures for solving the u and v momentum equations in the first stage are described. The computation procedures for solving the u and v momentum equations in the second stage consist of similar symmetrical expressions and have therefore been omitted from this subsection.

u momentum in the first stage

In this stage the discretized continuity equation and the discretized u momentum equation are solved simultaneously based on the model state at time t and the results of the preceding procedure which yields the v velocities at time $t+\frac{1}{2}\Delta t$. If the advective (and the viscosity) terms are omitted, the resulting discretized u momentum equation has the following structure (see formula (3.6)):

$$\frac{1}{\frac{1}{2}\Delta t}\left[u'_{m,n} - u_{m,n} \right] - \overline{f_{m,n} v'_{m,n}}^{\eta\xi} + \frac{g}{K^u_{m,n}}\left[\frac{\zeta'_{m+1,n} - \zeta'_{m,n}}{\Delta\xi} \right] + \frac{g}{C_u^2} \frac{u'_{m,n}\sqrt{(u'_{m,n})^2 + (\overline{v'}^{\eta\xi}_{m,n})^2}}{D^u_{m,n} + \overline{\zeta'}^{\xi}_{m,n}} = 0 \qquad (3.24)$$

The conservation of momentum in x direction contains three unknown variables. The advective term uu_x is discretized in this first stage as:

$$u'_{m,n} \frac{U_{m+1,n} - u_{m-1,n}}{2\Delta X} \qquad (3.25)$$

The difference u_x is approximated explicitly. This means using the u velocities at the old time level, which were determined in an earlier stage of the computation process. Consequently, the structure of equation (3.24) augmented with (3.25) remains the same; only the coefficients will alter. The cross-advective term vu_y is discretized in this stage as:

$$\overline{\overline{v'}}_{m,n} S^c_y(u_{m,n}) \qquad (3.26)$$

in which:

$$\overline{\overline{v}}_{m,n} = \overline{v}^{\eta\xi}_{m,n} = \tfrac{1}{4}\left[v_{m,n} + v_{m+1,n} + v_{m+1,n-1} + v_{m,n-1} \right]$$

$$S^c_y(u_{m,n}) = \frac{\left[u_{m,n+2} + 4u_{m,n+1} - 4u_{m,n-1} - u_{m,n-2} \right]}{12\Delta Y}$$

The difference u_y is approximated explicitly with a weighted central difference. For a discussion of the phase and amplitude errors of this approximation, see [Stelling, 1984]. In the preceding procedure these v velocities were computed and, due to the explicit approximation of u_y, the structure of equation (3.24) remains unaltered when equation (3.26) is added. With the exception of the boundary treatment, incorporating the advective terms at this stage of the computation process leaves the structure of the equations unimpaired.

For each row in the domain of the model all the u momentum equations and the continuity equations form a pentadiagonal matrix equation together with the boundary conditions.

$$\begin{array}{ccccccccccc}
\zeta & u_{m-2} & \zeta & & & & & & & & \\
\zeta & u & \zeta_{m-1} & u & \zeta & & & & & & \\
 & & \zeta & u_{m-1} & \zeta & & & & & & \\
 & & \zeta & u & \zeta_{m} & u & \zeta & & & & \\
 & & & & \zeta & u_{m} & \zeta & & & & \\
 & & & & \zeta & u & \zeta_{m+1} & u & \zeta & & \\
 & & & & & & \zeta & u_{m+1} & \zeta & &
\end{array}$$

(3.27)

The u contributions in the continuity equation are eliminated by means of the u momentum equation with a substitution.

There results for each row a tridiagonal matrix equation which consists solely of ζ contributions:

$$\begin{array}{ccccccc}
\zeta & \zeta_{m-1} & \zeta & & & & \\
 & \zeta & \zeta_{m} & \zeta & & & \\
 & & \zeta & \zeta_{m+1} & \zeta & & \\
 & & & \zeta & \zeta_{m+2} & \zeta &
\end{array} \qquad (3.28)$$

This matrix equation is solved with Gaussian elimination (double sweep method), [Stelling, 1984]. After here, the u momentum equation can be solved by simple substitution.

v momentum in the first stage

The v momentum equation in the first stage of the ADI method is solved on the basis of the solution of the model equations at time t. The term vv_y is discretized as:

$$v_{m,n}\frac{\left(v'_{m,n+1}-v'_{m,n-1}\right)}{2\Delta Y} \qquad (3.29)$$

Here the difference v_y is approximated implicitly: it is expressed in v velocities at the new time level. Therefore, the structure of the matrix equation will alter. Without the cross-advective term uv_x and the viscosity terms all the v momentum equations for a column in the domain form a tridiagonal matrix equation. As mentioned earlier, the well-known double sweep algorithm can be applied to perform this task.

Difficulties arise with the implicit approximation of the cross-advective term uv_x:

$$\bar{\bar{u}}_{m,n}\, S_x^u(v'_{m,n}) \tag{3.30}$$

in which:

$$\bar{\bar{u}}_{m,n} = \bar{u}^{\xi\eta}_{m,n} = \tfrac{1}{4}\left[u_{m,n} + u_{m-1,n} + u_{m-1,n+1} + u_{m,n+1}\right]$$

$$S_x^u(v_{m,n}) = \begin{cases} \dfrac{\left[3v_{m,n} - 4v_{m-1,n} + v_{m-2,n}\right]}{2\Delta X} & \text{if } \bar{\bar{u}}_{m,n} > 0 \\ \dfrac{\left[-3v_{m,n} + 4v_{m+1,n} - v_{m+2,n}\right]}{2\Delta X} & \text{if } \bar{\bar{u}}_{m,n} \le 0 \end{cases}$$

This is the so-called second order upwind approximation. These v velocities at the new time level are perpendicular to the ones which set up the tridiagonal structure. Therefore, these equations are solved column by column in a Gauss-Seidel iterative way. If a v velocity at the new time level from a nearby column is needed in the computation process and has not yet been computed, the most recent value should be taken instead. This enables the equations to be resolved again by solving tridiagonal matrices over grid lines.

This so-called predictor corrector procedure will now be explained in more detail. First of all the direction has to be determined: whether the tridiagonal systems over columns should be solved from left to right or from right to left. This depends on the dominant flow direction of u (defined by q') and the iteration number (defined by q).

$$q' = \begin{Bmatrix} 0 \text{ , if } \sum_{m,n} u > 0 \\ 1 \text{ , if } \sum_{m,n} u \le 0 \end{Bmatrix}$$

$$\delta(q, q') = \tfrac{1}{2}\left[1 + (-1)^{q+q'}\right] \tag{3.31}$$

$$v^{[0]} = v,\ v^{[2]} = v'$$

The second order upwind approximation ($q = 1, 2$) is:

$$S_x^u(\bar{\bar{u}}, v_{m,n}^{[q]}, v_{m,n}^{[q-1]}, \delta) = \begin{cases} \dfrac{\left[3v_{m,n}^{[q-\delta]} - 4v_{m-1,n}^{[q-\delta]} + v_{m-2,n}^{[q-\delta]}\right]}{2\Delta X} & \text{if } \bar{\bar{u}}_{m,n} > 0 \\ \dfrac{\left[-3v_{m,n}^{[q-1+\delta]} + 4v_{m+1,n}^{[q-1+\delta]} - v_{m+2,n}^{[q-1+\delta]}\right]}{2\Delta X} & \text{if } \bar{\bar{u}}_{m,n} \le 0 \end{cases} \quad (3.32)$$

The maximum number of iterations is two. These v momentum equations are solved column by column in the dominant flow direction of the u velocity. If the sign of u is constant then these equations are solved in one iteration, otherwise a second step is necessary. This step proceeds in the opposite direction.

V **V_{n-1}** **V**

V **V_n** **V** (3.33)

V **V_{n+1}** **V**

V **V_{n+2}** **V**

3.2.2.3. Adjoint Advective Terms

As mentioned earlier, advective terms only occur in both momentum equations. For each term at each stage in the computation process the adjoint counterpart will be deduced.

VV_Y

The v momentum equation is solved in the first stage of the ADI method. Here v_y is approximated implicitly. The discretisation of vv_y is as follows:

$$v_{m,n}\frac{\left(v'_{m,n+1} - v'_{m,n-1}\right)}{2\Delta Y} \quad (3.34)$$

Applying the variational formalism:

$$\Delta v_{m,n}\frac{\left(v'_{m,n+1} - v'_{m,n-1}\right)}{2\Delta Y} + v_{m,n}\frac{\left(\Delta v'_{m,n+1} - \Delta v'_{m,n-1}\right)}{2\Delta Y} \quad (3.35)$$

In constructing the adjoint v momentum equations the unknown terms with $\Delta v_{m,n}$ and $\Delta v'_{m,n}$ are important. The derivation will be done step by step for a fixed location (m,n) far away from the boundaries and impeded points. At the surrounding grid points the normal equations are solved.

- In the conservation of momentum in the y direction at point (m,n+1) the term vv_y occurs as:

$$v_{m,n+1}\frac{\left(v'_{m,n+2}-v'_{m,n}\right)}{2\Delta Y} \tag{3.36}$$

Introduce Lagrange multipliers and apply variational formalism:

$$(\nu_v)'_{m,n+1}\left\{\cdots\left(-\frac{v_{m,n+1}}{2\Delta Y}\right)\Delta v'_{m,n}+\left(\frac{v'_{m,n+2}-v'_{m,n}}{2\Delta Y}\right)\Delta v_{m,n+1}+\left(\frac{v_{m,n+1}}{2\Delta Y}\right)\Delta v'_{m,n+2}\cdots\right\} \tag{3.37}$$

Remark: the dots in equation (3.37) and the following equations denote the other (non-advective) adjoint terms.

- In the conservation of momentum in the y direction at point (m,n-1) the term vv_y occurs as:

$$v_{m,n-1}\frac{\left(v'_{m,n}-v'_{m,n-2}\right)}{2\Delta Y} \tag{3.38}$$

Introduce Lagrange multipliers and apply variational formalism:

$$(\nu_v)'_{m,n-1}\left\{\cdots\left(-\frac{v_{m,n-1}}{2\Delta Y}\right)\Delta v'_{m,n-1}+\left(\frac{v'_{m,n}-v'_{m,n-2}}{2\Delta Y}\right)\Delta v_{m,n-1}+\left(\frac{v_{m,n-1}}{2\Delta Y}\right)\Delta v'_{m,n}\cdots\right\} \tag{3.39}$$

In (3.35), (3.37) and (3.39) we focus on $\Delta v_{m,n}$ and $\Delta v'_{m,n}$, since we are interested in the adjoint conservation of momentum in y direction at location (m,n).

In (3.39): $(\nu_v)'_{m,n-1}\left\{\cdots\left(\frac{v_{m,n-1}}{2\Delta Y}\right)\Delta v'_{m,n}\cdots\right\}$ (3.40)

$$\text{In (3.35): } (\nu_v)'_{m,n} \left\{ \cdots \Delta v_{m,n} \left(\frac{v'_{mn,+1} - v'_{m,n-1}}{2\Delta Y} \right) \cdots \right\} \tag{3.41}$$

$$\text{In (3.37): } (\nu_v)'_{m,n+1} \left\{ \cdots \left(-\frac{v_{m,n+1}}{2\Delta Y} \right) \Delta v'_{m,n} \cdots \right\} \tag{3.42}$$

A fragment of the adjoint v momentum equations can be determined using this, as will be demonstrated at the end of this section. In the second stage the v momentum equation is solved simultaneously with the conservation of mass. In this second stage of the ADI method, v_y in the conservation of momentum in y direction for location (m,n) is approximated explicitly. The discretization of vv_y is:

$$v''_{m,n} \frac{\left(v'_{m,n+1} - v'_{m,n-1} \right)}{2\Delta Y} \tag{3.43}$$

Applying the variational formalism again:

$$\Delta v''_{m,n} \frac{\left(v'_{m,n+1} - v'_{m,n-1} \right)}{2\Delta Y} + v''_{m,n} \frac{\left(\Delta v'_{m,n+1} - \Delta v'_{m,n-1} \right)}{2\Delta Y} \tag{3.44}$$

- In the v momentum equation for location (m,n+1) in this second stage vv_y occurs as:

$$v''_{m,n+1} \frac{\left(v'_{m,n+2} - v'_{m,n} \right)}{2\Delta Y} \tag{3.45}$$

  Introduce Lagrange multipliers and apply variational formalism:

$$(\nu_v)''_{m,n+1} \left\{ \cdots \left(-\frac{v''_{m,n+1}}{2\Delta Y} \right) \Delta v'_{m,n} + \left(\frac{v'_{m,n+2} - v_{m',n}}{2\Delta Y} \right) \Delta v''_{m,n+1} + \left(\frac{v''_{m,n+1}}{2\Delta Y} \right) \Delta v'_{m,n+2} \cdots \right\} \tag{3.46}$$

- In the conservation of momentum in the y direction at point (m,n-1) in the second stage the term vv_y occurs as:

$$v''_{m,n-1}\frac{\left(\ v'_{m,n} - v'_{m,n-2}\ \right)}{2\Delta Y} \tag{3.47}$$

Introduce Lagrange multipliers and apply variational formalism:

$$(\nu_v)''_{m,n-1}\left\{\ \cdots\left(\ -\frac{v''_{m,n-1}}{2\Delta Y}\ \right)\Delta v'_{m,n-2} + \left(\ \frac{v'_{m,n} - v'_{m,n-2}}{2\Delta Y}\ \right)\Delta v''_{m,n-1} + \left(\ \frac{v''_{m,n-1}}{2\Delta Y}\ \right)\Delta v'_{m,n}\ \cdots\ \right\} \tag{3.48}$$

In (3.44), (3.46) and (3.48) we focus on the terms with $\Delta v'_{m,n}$ and $\Delta v''_{m,n}$. The latter can be used for constructing the adjoint equation for $v_{m,n}$.

In (3.48): $(\nu_v)''_{m,n-1}\left\{\ \cdots\left(\ \frac{v''_{m,n-1}}{2\Delta Y}\ \right)\Delta v'_{m,n}\ \cdots\ \right\}$ (3.49)

In (3.44): $(\nu_v)''_{m,n}\left\{\ \cdots\Delta v''_{m,n}\left(\ \frac{v'_{m,n+1} - v'_{m,n-1}}{2\Delta Y}\ \right)\cdots\ \right\}$ (3.50)

In (3.46): $(\nu_v)''_{m,n+1}\left\{\ \cdots\left(\ -\frac{v''_{m,n+1}}{2\Delta Y}\ \right)\Delta v'_{m,n}\ \cdots\ \right\}$ (3.51)

Finally some parts of the adjoint v momentum equations can be determined. To compute the gradient the cost function has been augmented with additional terms, each of which is the product of an undetermined multiplier and a model equation. After differentiating this Lagrange function the summation is rearranged: some additional terms are now the product of an unknown derivative and an equation in Lagrange multipliers. In the other additional terms no unknown derivatives of discrete model variables occur. This procedure enables the derivative of the cost function to be evaluated, providing the Lagrange multipliers satisfy the adjoint equations.

Rearranging the summation in (3.40), (3.41), (3.42), (3.49), (3.50) and (3.51) yields:

$$\Delta v'_{m,n}\left\{ \cdots \frac{\left(v_{m,n-1}(\nu_v)'_{m,n-1} - v_{m,n+1}(\nu_v)'_{m,n+1} \right)}{2\Delta Y} + \frac{\left(v''_{m,n-1}(\nu_v)''_{m,n-1} - v''_{m,n+1}(\nu_v)''_{m,n+1} \right)}{2\Delta Y} \cdots \right\} \tag{3.52}$$

$$\Delta v_{m,n}\left\{ \cdots (\nu_v)'_{m,n} \frac{\left(v'_{m,n+1} - v'_{m,n-1} \right)}{2\Delta Y} + (\nu_v)_{m,n} \frac{\left(v^{-'}_{m,n+1} - v^{-'}_{m,n-1} \right)}{2\Delta Y} \cdots \right\} \tag{3.53}$$

where '$^{-'}$' denotes the state variable at time t-½Δt.

The expressions between braces are part of the adjoint v momentum equations, which are solved in the computing procedures in the first and second stage.

VU_Y

This cross advective term occurs in the conservation of momentum in x direction. In the first stage of the ADI method u_y is approximated by a weighted central difference (explicit). In the second stage another difference scheme is used, namely a second order upwind difference (implicit). The phase and amplitude errors of the combined approximation are discussed in [Stelling, 1984]. At this first stage in the u momentum equation at location (m,n) the term vu_y is discretized as follows:

$$\overline{\overline{v'}}_{m,n}\, S_y^c(u_{m,n}) \tag{3.54}$$

in which:

$$\overline{\overline{v}}_{m,n} = \overline{v}^{\eta\xi}_{m,n} = \tfrac{1}{4}\left[v_{m,n} + v_{m+1,n} + v_{m+1,n-1} + v_{m,n-1} \right]$$

$$S_y^c(u_{m,n}) = \frac{\left[u_{m,n+2} + 4u_{m,n+1} - 4u_{m,n-1} - u_{m,n-2} \right]}{12\Delta Y}$$

Applying variational formalism yields:

$$\begin{aligned} &\Delta u_{m,n+2}\frac{\overline{\overline{v'}}_{m,n}}{12\Delta Y} + \Delta u_{m,n+1}\frac{4\overline{\overline{v'}}_{m,n}}{12\Delta Y} - \\ &\Delta u_{m,n-1}\frac{4\overline{\overline{v'}}_{m,n}}{12\Delta Y} - \Delta u_{m,n-2}\frac{\overline{\overline{v'}}_{m,n}}{12\Delta Y} + \\ &\Delta v'_{m,n}\,\tfrac{1}{4}S_y^c(u_{m,n}) + \Delta v'_{m+1,n}\,\tfrac{1}{4}S_y^c(u_{m,n}) + \\ &\Delta v'_{m+1,n-1}\,\tfrac{1}{4}S_y^c(u_{m,n}) + \Delta v'_{m,n-1}\,\tfrac{1}{4}S_y^c(u_{m,n}) \end{aligned} \tag{3.55}$$

Equal to:

$$\overline{\overline{v'}}_{m,n}\, S_y^c(\Delta u_{m,n}) + \Delta\overline{\overline{v'}}_{m,n}\, S_y^c(u_{m,n})$$

In this expression several derivatives of discrete model variables are found located at different grid points. The entire formula has to be multiplied by the corresponding adjoint variable. To build up the adjoint equation this summation of products has to be rearranged: one derivative of a discrete model variable located at one grid point has to be multiplied by a formula in adjoint variables.

First of all we concentrate on the u momentum equations at different locations in which terms with $\Delta u_{m,n}$ are found, descended from this cross advective term solved in the first stage of the ADI method.

- In the first stage in the conservation of momentum in x direction at location (m,n-2), after introducing Lagrange multipliers and applying the variational formalism, we find:

$$(\nu_u)'_{m,n-2}\left\{\cdots\left(\frac{\overline{\overline{v'}}_{m,n-2}}{12\Delta Y}\right)\Delta u_{m,n}\cdots\right\} \tag{3.56}$$

- In the first stage in the conservation of momentum in x direction at location (m,n-1), after introducing Lagrange multipliers and applying the variational formalism, we find:

$$(\nu_u)'_{m,n-1}\left\{\cdots\left(\frac{4\overline{\overline{v'}}_{m,n-1}}{12\Delta Y}\right)\Delta u_{m,n}\cdots\right\} \tag{3.57}$$

- In the first stage in the conservation of momentum in x direction at location (m,n+1), after introducing Lagrange multipliers and applying the variational formalism, we find:

$$(\nu_u)'_{m,n+1}\left\{\cdots\left(\frac{-4\overline{\overline{v'}}_{m,n+1}}{12\Delta Y}\right)\Delta u_{m,n}\cdots\right\} \tag{3.58}$$

- In the first stage in the conservation of momentum in x direction at location (m,n+2), after introducing Lagrange multipliers and applying the variational formalism, we find:

$$(\nu_u)'_{m,n+2}\left\{\cdots\left(\frac{-\overline{\overline{v'}}_{m,n+2}}{12\Delta Y}\right)\Delta u_{m,n}\cdots\right\} \tag{3.59}$$

Finally by rearranging the terms in the summation a part of the adjoint u momentum equation can be determined.

$$\Delta u_{m,n}\left\{\cdots(\nu_u)'_{m,n-2}\left(\frac{\overline{\overline{v'}}_{m,n-2}}{12\Delta Y}\right)+(\nu_u)'_{m,n-1}\left(\frac{4\overline{\overline{v'}}_{m,n-1}}{12\Delta Y}\right)-(\nu_u)'_{m,n+1}\left(\frac{4\overline{\overline{v'}}_{m,n+1}}{12\Delta Y}\right)-(\nu_u)'_{m,n+2}\left(\frac{\overline{\overline{v'}}_{m,n+2}}{12\Delta Y}\right)\cdots\right\} \tag{3.60}$$

The expression between braces is part of the adjoint conservation of momentum in x direction, which is solved in the computation procedure of the second stage.

Now we focus on the u momentum equations in those locations in which terms with $\Delta v'_{m,n}$ are found, descended from this cross-advective term solved in the first stage of the ADI method.

- In the first stage of the conservation of momentum in x direction at location (m,n), after introducing Lagrange multipliers and applying the variational formalism, we find:

$$(\nu_u)'_{m,n}\left\{ \cdots \tfrac{1}{4} S_y^c(u_{m,n})\Delta v'_{m,n} \cdots \right\} \qquad (3.61)$$

- In the first stage of the conservation of momentum in x direction at location (m-1,n), after introducing Lagrange multipliers and applying the variational formalism, we find:

$$(\nu_u)'_{m-1,n}\left\{ \cdots \tfrac{1}{4} S_y^c(u_{m-1,n})\Delta v'_{m,n} \cdots \right\} \qquad (3.62)$$

- In the first stage of the conservation of momentum in x direction at location (m-1,n+1), after introducing Lagrange multipliers and applying the variational formalism, we find:

$$(\nu_u)'_{m-1,n+1}\left\{ \cdots \tfrac{1}{4} S_y^c(u_{m-1,n+1})\Delta v'_{m,n} \cdots \right\} \qquad (3.63)$$

- In the first stage of the conservation of momentum in x direction at location (m,n+1), after introducing Lagrange multipliers and applying the variational formalism, we find:

$$(\nu_u)'_{m,n+1}\left\{ \cdots \tfrac{1}{4} S_y^c(u_{m,n+1})\Delta v'_{m,n} \cdots \right\} \qquad (3.64)$$

Finally by rearranging the terms in the summation, we obtain:

$$\Delta v'_{m,n}\left\{ \cdots (\nu_u)'_{m,n}\tfrac{1}{4}S_y^c(u_{m,n}) + (\nu_u)'_{m-1,n}\tfrac{1}{4}S_y^c(u_{m-1,n}) + (\nu_u)'_{m-1,n+1}\tfrac{1}{4}S_y^c(u_{m-1,n+1}) + (\nu_u)'_{m,n+1}\tfrac{1}{4}S_y^c(u_{m,n+1}) \cdots \right\} \qquad (3.65)$$

The expression between braces is part of the adjoint conservation of momentum in y direction, which is solved in the computation procedure of the first stage.

In the second stage the difference u_y is approximated by a second order upwind difference (implicit). This results in the following approximation of vu_y:

$$\overline{\overline{v'}}_{m,n}\, S_y^u(u'_{m,n}) \tag{3.66}$$

in which:

$$\overline{\overline{v}}_{m,n} = \overline{v}^{\eta\xi}_{m,n} = \tfrac{1}{4}\left[v_{m,n} + v_{m+1,n} + v_{m+1,n-1} + v_{m,n-1} \right]$$

$$S_y^u(u_{m,n}) = \begin{cases} \dfrac{\left[3u_{m,n} - 4u_{m,n-1} + u_{m,n-2} \right]}{2\Delta Y} & \text{if } \overline{\overline{v'}}_{m,n} > 0 \\ \dfrac{\left[-3u_{m,n} + 4u_{m,n+1} - u_{m,n+2} \right]}{2\Delta Y} & \text{if } \overline{\overline{v'}}_{m,n} \le 0 \end{cases}$$

Differentiating this expression with respect to an arbitrary model parameter yields:

$$\begin{aligned} &\Delta v'_{m,n}\, \tfrac{1}{4} S_y^u(u''_{m,n}) + \Delta v'_{m+1,n}\, \tfrac{1}{4} S_y^u(u''_{m,n}) + \\ &\Delta v'_{m+1,n-1}\, \tfrac{1}{4} S_y^u(u''_{m,n}) + \Delta v'_{m,n-1}\, \tfrac{1}{4} S_y^u(u''_{m,n}) \end{aligned} \tag{3.67}$$

added to:

$$\Delta u''_{m,n} \left(\frac{3\overline{\overline{v'}}_{m,n}}{2\Delta Y} \right) + \Delta u''_{m,n-1} \left(\frac{-4\overline{\overline{v'}}_{m,n}}{2\Delta Y} \right) + \Delta u''_{m,n-2} \left(\frac{\overline{\overline{v'}}_{m,n}}{2\Delta Y} \right) \quad \text{if } \overline{\overline{v'}}_{m,n} > 0$$

or added to:

$$\Delta u''_{m,n} \left(\frac{-3\overline{\overline{v'}}_{m,n}}{2\Delta Y} \right) + \Delta u'_{m,n+1} \left(\frac{4\overline{\overline{v'}}_{m,n}}{2\Delta Y} \right) + \Delta u''_{m,n+2} \left(\frac{-\overline{\overline{v'}}_{m,n}}{2\Delta Y} \right) \quad \text{if } \overline{\overline{v'}}_{m,n} \le 0$$

Equal to:

$$\Delta\overline{\overline{v'}}_{m,n}\; S_y^u(u''_{m,n}) + \overline{\overline{v'}}_{m,n}\; S_y^u(\Delta u''_{m,n})$$

First we concentrate on the counterpart of this term in the adjoint v momentum equation. Therefore, we examine the u momentum equations solved in the second stage of the ADI method at the locations (m,n), (m-1,n), (m-1,n+1), (m,n+1): these equations contain factors with the differential $\Delta v'_{m,n}$ (after introducing Lagrange multipliers and applying variational formalism). Assembling yields:

$$\Delta v'_{m,n} \left\{ \cdot\cdot (\nu_u)'_{m,n} \frac{1}{4} S_y^u(u''_{m,n}) + (\nu_u)''_{m-1,n} \frac{1}{4} S_y^u(u''_{m-1,n}) + (\nu_u)''_{m-1,n+1} \frac{1}{4} S_y^u(u''_{m-1,n+1}) + (\nu_u)''_{m,n+1} \frac{1}{4} S_y^u(u''_{m,n+1}) \cdot\cdot \right\} \tag{3.68}$$

The expression between braces contributes to the adjoint v momentum equation which is solved at the first stage. It only affects the right-hand side of the equation, not the matrix structure.

The appearance of the differentials $\Delta u''$ in equation (3.67) also implies contributions to the adjoint u momentum equation solved in the second stage. Since the discretisation of u_y is dependent on the flow direction of the v velocity, two situations have to be distinguished at each location. After differentiating we focus on the equations at the locations which contain factors with the differential $\Delta u''_{m,n}$.

- At location (m,n+2) in this stage, vu_y is discretized as $\overline{\overline{v'}}_{m,n+2} S_y^u(u''_{m,n+2})$. Consequently, we find:

$$\Delta u''_{m,n} \left(\frac{\overline{\overline{v'}}_{m,n+2}}{2\Delta Y} \right) \quad \text{if } \overline{\overline{v'}}_{m,n+2} > 0,$$
$$0 \quad \text{if } \overline{\overline{v'}}_{m,n+2} \le 0 \tag{3.69}$$

- At location (m,n+1) in this stage, vu_y is discretized as $\overline{\overline{v'}}_{m,n+1} S_y^u(u''_{m,n+1})$. Consequently, we find:

$$\Delta u''_{m,n} \begin{cases} \left(\dfrac{-4\overline{\overline{v'}}_{m,n+1}}{2\Delta Y} \right) & \text{if } \overline{\overline{v'}}_{m,n+1} > 0, \\ 0 & \text{if } \overline{\overline{v'}}_{m,n+1} \le 0 \end{cases} \qquad (3.70)$$

- At location (m,n) in this stage, vu_y is discretized as $\overline{\overline{v'}}_{m,n} S_y^u(u''_{m,n})$. Consequently, we find:

$$\Delta u''_{m,n} \begin{cases} \left(\dfrac{3\overline{\overline{v'}}_{m,n}}{2\Delta Y} \right) & \text{if } \overline{\overline{v'}}_{m,n} > 0, \\ \left(\dfrac{-3\overline{\overline{v'}}_{m,n}}{2\Delta Y} \right) & \text{if } \overline{\overline{v'}}_{m,n} \le 0 \end{cases} \qquad (3.71)$$

- At location (m,n-1) in this stage, vu_y is discretized as $\overline{\overline{v'}}_{m,n-1} S_y^u(u''_{m,n-1})$. Consequently, we find:

$$\Delta u''_{m,n} \begin{cases} 0 & \text{if } \overline{\overline{v'}}_{m,n-1} > 0, \\ \left(\dfrac{4\overline{\overline{v'}}_{m,n-1}}{2\Delta Y} \right) & \text{if } \overline{\overline{v'}}_{m,n-1} \le 0 \end{cases} \qquad (3.72)$$

- At location (m,n-2) in this stage, vu_y is discretized as $\overline{\overline{v'}}_{m,n-2} S_y^u(u'_{m,n-2})$. Consequently, we find:

$$\Delta u''_{m,n} \begin{cases} 0 & \text{if } \overline{\overline{v'}}_{m,n-2} > 0, \\ \left(\dfrac{-\overline{\overline{v'}}_{m,n-2}}{2\Delta Y} \right) & \text{if } \overline{\overline{v'}}_{m,n-2} \le 0 \end{cases} \qquad (3.73)$$

Since the computation procedure in the second stage performs the computation of (ν_u) to make Δu vanish, the expressions above have to be translated in time; this means that they can be derived from the same expressions in the previous stage.

It follows from equations (3.69) to (3.73) that a part of the adjoint equation associated with $\Delta u_{m,n}$ looks like:

$$(\nu_u)_{m,n+2}\left(\frac{\overset{=-'}{v_{m,n+2}}}{2\Delta Y}\right) \qquad if \ \overset{=-'}{v_{m,n+2}} > 0 \tag{3.74}$$

$$+(\nu_u)_{m,n+1}\left(\frac{\overset{=-'}{-4v_{m,n+1}}}{2\Delta Y}\right) \qquad if \ \overset{=-'}{v_{m,n+1}} > 0$$

$$+(\nu_u)_{m,n}\left(\frac{\overset{=-'}{3v_{m,n}}}{2\Delta Y}\right) \qquad if \ \overset{=-'}{v_{m,n}} > 0\,,$$

or

$$+(\nu_u)_{m,n}\left(\frac{\overset{=-'}{-3v_{m,n}}}{2\Delta Y}\right) \qquad if \ \overset{=-'}{v_{m,n}} \le 0$$

$$+(\nu_u)_{m,n-1}\left(\frac{\overset{=-'}{4v_{m,n-1}}}{2\Delta Y}\right) \qquad if \ \overset{=-'}{v_{m,n-1}} \le 0$$

$$+(\nu_u)_{m,n-2}\left(\frac{\overset{=-'}{-v_{m,n-2}}}{2\Delta Y}\right) \qquad if \ \overset{=-'}{v_{m,n-2}} \le 0$$

These adjoint u variables at time t are perpendicular to the ones in in the computation procedure in the second stage which set up the tridiagonal structure, if the advective terms were ignored. Therefore, in imitation of WAQUA, an iterative solution scheme is proposed: a Gauss-Seidel or Jacobi method. This allows the equations to still be resolved by solving tridiagonal matrices over grid lines, because in the 'adjoint' cross advective part the latest computed adjoint u velocities (Gauss-Seidel) or the ones originating from the previous iteration level (Jacobi) are used.

UU_X

The u momentum equation and the conservation of mass are simultaneously solved in the first stage of the ADI method. Here the difference u_x is approximated explicitly. The discretization of uu_x in this equation is as follows:

$$u'_{m,n}\frac{\left(u_{m+1,n}-u_{m-1,n}\right)}{2\Delta X} \tag{3.75}$$

After differentiating:

$$\Delta u'_{m,n}\frac{\left(u_{m+1,n}-u_{m-1,n}\right)}{2\Delta X}+u'_{m,n}\frac{\left(\Delta u_{m+1,n}-\Delta u_{m-1,n}\right)}{2\Delta X} \tag{3.76}$$

In the second stage of the ADI method the difference u_x is approximated implicitly. Here the discretization of uu_x is:

$$u'_{m,n}\frac{\left(u''_{m+1,n}-u''_{m-1,n}\right)}{2\Delta X} \tag{3.77}$$

After differentiating:

$$\Delta u'_{m,n}\frac{\left(u''_{m+1,n}-u''_{m-1,n}\right)}{2\Delta X}+u'_{m,n}\frac{\left(\Delta u''_{m+1,n}-\Delta u''_{m-1,n}\right)}{2\Delta X} \tag{3.78}$$

Since the adjoint treatment is completely analogous to the term vv_y, only the most important formulas will be given. We focus on those u momentum equations at different locations in which terms with $\Delta u_{m,n}$ and $\Delta u'_{m,n}$ are found, after applying the variational formalism and introducing the proper Lagrange multipliers for equations (3.76) and (3.78).

- In the first stage in the u momentum equation at location (m-1,n) we find:

$$(\nu_u)'_{m-1,n}\left\{\cdots\left(\frac{u'_{m-1,n}}{2\Delta X}\right)\Delta u_{m,n}\cdots\right\} \tag{3.79}$$

- In the first stage in the u momentum equation at location (m,n) we find:

$$(\nu_u)'_{m,n} \left\{ \cdots \Delta u'_{m,n} \left(\frac{u_{m+1,n} - u_{m-1,n}}{2\Delta X} \right) \cdots \right\} \tag{3.80}$$

- In the first stage in the u momentum equation at location (m+1,n) we find:

$$(\nu_u)'_{m+1,n} \left\{ \cdots \left(- \frac{u'_{m+1,n}}{2\Delta X} \right) \Delta u_{m,n} \cdots \right\} \tag{3.81}$$

- In the second stage in the u momentum equation at location (m-1,n) we find:

$$(\nu_u)''_{m-1,n} \left\{ \cdots \left(\frac{u'_{m-1,n}}{2\Delta X} \right) \Delta u''_{m,n} \cdots \right\} \tag{3.82}$$

- In the second stage in the u momentum equation at location (m,n) we find:

$$(\nu_u)''_{m,n} \left\{ \cdots \Delta u'_{m,n} \left(\frac{u''_{m+1,n} - u''_{m-1,n}}{2\Delta X} \right) \cdots \right\} \tag{3.83}$$

- In the second stage in the u momentum equation at location (m+1,n) we find:

$$(\nu_u)''_{m+1,n} \left\{ \cdots \left(- \frac{u'_{m+1,n}}{2\Delta X} \right) \Delta u''_{m,n} \cdots \right\} \tag{3.84}$$

Rearranging the summation in equations (3.79) to (3.84) and thereby constructing parts of the adjoint equations yields:

$$\Delta u'_{m,n} \left\{ \cdots (\nu_u)'_{m,n} \frac{\left(u_{m+1,n} - u_{m-1,n} \right)}{2\Delta X} + (\nu_u)''_{m,n} \frac{\left(u''_{m+1,n} - u''_{m-1,n} \right)}{2\Delta X} \cdots \right\} \tag{3.85}$$

$$\Delta u_{m,n}\left\{ \cdots \frac{\left(u'_{m-1,n}(\nu_u)'_{m-1,n} - u'_{m+1,n}(\nu_u)'_{m+1,n} \right)}{2\Delta X} + \frac{\left(u'_{m-1,n}(\nu_u)_{m-1,n} - u'_{m+1,n}(\nu_u)_{m+1,n} \right)}{2\Delta X} \cdots \right\} \tag{3.86}$$

The expressions between braces are part of the adjoint u momentum equations which are solved in the computation procedures in the first stage.

UV_X

This cross advective term occurs in the v momentum equation. In the first stage of the ADI method a second order upwind difference is used to approximate v_x implicitly. In the second stage a weighted central difference approximates v_x explicitly. The treatment is analogous to the other cross-advective term vu_y in the u momentum equation. Only the important formulas are presented below.

In the first stage the difference v_x is approximated by a second order upwind difference (implicit). This results in the following approximation of uv_x:

$$\bar{\bar{u}}_{m,n}\, S_x^u(v'_{m,n}) \tag{3.87}$$

in which:

$$\bar{\bar{u}}_{m,n} = \bar{u}^{\xi\eta}_{m,n} = \tfrac{1}{4}\left[u_{m,n} + u_{m-1,n} + u_{m-1,n+1} + u_{m,n+1}\right]$$

$$S_x^u(v_{m,n}) = \begin{cases} \dfrac{\left[3v_{m,n} - 4v_{m-1,n} + v_{m-2,n}\right]}{2\Delta X} & \text{if } \bar{\bar{u}}_{m,n} > 0 \\ \dfrac{\left[-3v_{m,n} + 4v_{m+1,n} - v_{m+2,n}\right]}{2\Delta X} & \text{if } \bar{\bar{u}}_{m,n} \le 0 \end{cases}$$

Differentiating this expression with respect to an arbitrary model parameter yields:

$$\Delta u_{m,n}\,\tfrac{1}{4}S_x^u(v'_{m,n}) + \Delta u_{m-1,n}\,\tfrac{1}{4}S_x^u(v'_{m,n}) + \Delta u_{m-1,n+1}\,\tfrac{1}{4}S_x^u(v'_{m,n}) + \Delta u_{m,n+1}\,\tfrac{1}{4}S_x^u(v'_{m,n}) \tag{3.88}$$

added to:

$$\Delta v'_{m,n}\left(\frac{3\bar{u}_{m,n}}{2\Delta X}\right) + \Delta v_{m'-1,n}\left(\frac{-4\bar{u}_{m,n}}{2\Delta X}\right) + \Delta v'_{m-2,n}\left(\frac{\bar{u}_{m,n}}{2\Delta X}\right) \qquad \text{if } \bar{u}_{m,n} > 0$$

or added to:

$$\Delta v'_{m,n}\left(\frac{-3\bar{u}_{m,n}}{2\Delta X}\right) + \Delta v'_{m+1,n}\left(\frac{4\bar{u}_{m,n}}{2\Delta X}\right) + \Delta v'_{m+2,n}\left(\frac{-\bar{u}_{m,n}}{2\Delta X}\right) \qquad \text{if } \bar{u}_{m,n} \le 0$$

Equal to:

$$\Delta\bar{u}_{m,n}\;S_x^u(v'_{m,n}) + \bar{u}_{m,n}\;S_x^u(\Delta v'_{m,n})$$

First we concentrate on the counterpart of this term in the adjoint u momentum equation. Therefore, we examine the v momentum equations solved in the first stage of the ADI method at the locations (m,n), (m+1,n), (m+1,n-1), (m,n-1): these equations contain factors with the differential $\Delta u_{m,n}$ (after introducing Lagrange multipliers and applying variational formalism). Assembling yields:

$$\Delta u_{m,n}\Big\{\;\cdots(\nu_v)'_{m,n}\,\tfrac{1}{4}S_x^u(v'_{m,n}) + (\nu_v)'_{m+1,n}\,\tfrac{1}{4}S_x^u(v'_{m+1,n}) + (\nu_v)'_{m+1,n-1}\,\tfrac{1}{4}S_x^u(v'_{m+1,n-1}) + (\nu_v)'_{m,n-1}\,\tfrac{1}{4}S_x^u(v'_{m,n-1})\cdots\;\Big\} \tag{3.89}$$

The expression between braces contributes to the adjoint u momentum equation which is solved in the computation procedure of the second stage. It only affects the right-hand side.

The appearance of the differentials $\Delta v'$ in equation (3.88) also implies contributions to the adjoint v momentum equation

solved in the computation procedure of the first stage. Since the discretization of v_x is dependent on the flow direction of the u velocity, two situations have to be distinguished at each location. After differentiating we focus on the equations at the locations which contain factors with the differential $\Delta v'_{m,n}$.

- At location (m-2,n) in this stage, uv_x is discretized as $\bar{\bar{u}}_{m-2,n} S_x^u(v'_{m-2,n})$. Consequently, we find:

$$\begin{cases} 0 & \text{if } \bar{\bar{u}}_{m-2,n} > 0, \\ \Delta v'_{m,n} \left(\dfrac{-\bar{\bar{u}}_{m-2,n}}{2\Delta X} \right) & \text{if } \bar{\bar{u}}_{m-2,n} \le 0 \end{cases} \qquad (3.90)$$

- At location (m-1,n) in this stage, uv_x is discretized as $\bar{\bar{u}}_{m-1,n} S_x^u(v'_{m-1,n})$. Consequently, we find:

$$\begin{cases} 0 & \text{if } \bar{\bar{u}}_{m-1,n} > 0, \\ \Delta v'_{m,n} \left(\dfrac{4\bar{\bar{u}}_{m-1,n}}{2\Delta X} \right) & \text{if } \bar{\bar{u}}_{m-1,n} \le 0 \end{cases} \qquad (3.91)$$

- At location (m,n) in this stage, uv_x is discretized as $\bar{\bar{u}}_{m,n} S_x^u(v'_{m,n})$. Consequently, we find:

$$\begin{cases} \Delta v'_{m,n} \left(\dfrac{3\bar{\bar{u}}_{m,n}}{2\Delta X} \right) & \text{if } \bar{\bar{u}}_{m,n} > 0, \\ \Delta v'_{m,n} \left(\dfrac{-3\bar{\bar{u}}_{m,n}}{2\Delta X} \right) & \text{if } \bar{\bar{u}}_{m,n} \le 0 \end{cases} \qquad (3.92)$$

- At location (m+1,n) in this stage, uv_x is discretized as $\bar{\bar{u}}_{m+1,n} S_x^u(v'_{m+1,n})$. Consequently, we find:

$$\begin{cases} \Delta v'_{m,n} \left(\dfrac{-4\bar{\bar{u}}_{m+1,n}}{2\Delta X} \right) & \text{if } \bar{\bar{u}}_{m+1,n} > 0, \\ 0 & \text{if } \bar{\bar{u}}_{m+1,n} \le 0 \end{cases} \qquad (3.93)$$

- At location (m+2,n) in this stage, uv_x is discretized as $\bar{\bar{u}}_{m+2,n} S_x^u(v'_{m+2,n})$. Consequently, we find:

$$\begin{cases} \Delta v'_{m,n} \left(\dfrac{\bar{\bar{u}}_{m+2,n}}{2\Delta X} \right) & \text{if } \bar{\bar{u}}_{m+2,n} > 0, \\ 0 & \text{if } \bar{\bar{u}}_{m+2,n} \le 0 \end{cases} \qquad (3.94)$$

It follows from equations (3.91) to (3.94) that a part of the adjoint equation associated with $\Delta v'_{m,n}$ looks like:

$$(\nu_v)'_{m-2,n} \left(\frac{-\bar{\bar{u}}_{m-2,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m-2,n} \le 0 \qquad (3.95)$$

$$+ (\nu_v)'_{m-1,n} \left(\frac{4\bar{\bar{u}}_{m-1,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m-1,n} \le 0$$

$$+ (\nu_v)'_{m,n} \left(\frac{-3\bar{\bar{u}}_{m,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m,n} \le 0,$$

or

$$+ (\nu_v)'_{m,n} \left(\frac{3\bar{\bar{u}}_{m,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m,n} > 0$$

$$+ (\nu_v)'_{m+1,n} \left(\frac{-4\bar{\bar{u}}_{m+1,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m+1,n} > 0$$

$$+ (\nu_v)'_{m+2,n} \left(\frac{\bar{\bar{u}}_{m+2,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m+2,n} > 0$$

These adjoint v variables at time t+½Δt are perpendicular to the ones in the computation procedure of the first stage which set up the tridiagonal structure, if the advective terms were ignored. Therefore, in imitation of WAQUA, an iterative solution scheme is proposed: a Gauss-Seidel or Jacobi method. This allows the equations to still be resolved by solving tridiagonal matrices over grid lines, because in the 'adjoint' cross advective part the latest computed adjoint v velocities (Gauss-Seidel) or the ones originating from the previous iteration level (Jacobi) are used.

The weighted central difference of uv_x at the second stage looks like:

$$\overline{\overline{u''}}_{m,n}\, S_x^c(v'_{m,n}) \tag{3.96}$$

in which:

$$\overline{\overline{u}}_{m,n} = \overline{\overline{u}}^{\xi\eta}_{m,n} = \tfrac{1}{4}\left[u_{m,n} + u_{m-1,n} + u_{m-1,n+1} + u_{m,n+1}\right]$$

$$S_x^c(v_{m,n}) = \frac{\left[v_{m+2,n} + 4v_{m+1,n} - 4v_{m-1,n} - v_{m-2,n}\right]}{12\Delta X}$$

Applying variational formalism yields:

$$\begin{aligned}
&\Delta v'_{m+2,n}\,\frac{\overline{\overline{u''}}_{m,n}}{12\Delta X} + \Delta v'_{m+1,n}\,\frac{4\overline{\overline{u''}}_{m,n}}{12\Delta X} - \\
&\Delta v'_{m-1,n}\,\frac{4\overline{\overline{u''}}_{m,n}}{12\Delta X} - \Delta v'_{m-2,n}\,\frac{\overline{\overline{u''}}_{m,n}}{12\Delta X} + \\
&\Delta u''_{m,n}\,\tfrac{1}{4}S_x^c(v'_{m,n}) + \Delta u''_{m-1,n}\,\tfrac{1}{4}S_x^c(v'_{m,n}) + \\
&\Delta u''_{m-1,n+1}\,\tfrac{1}{4}S_x^c(v'_{m,n}) + \Delta u''_{m,n+1}\,\tfrac{1}{4}S_x^c(v'_{m,n})
\end{aligned} \tag{3.97}$$

which equals:

$$\overline{\overline{u''}}_{m,n}\, S_x^c(\Delta v'_{m,n}) + \Delta\overline{\overline{u''}}_{m,n}\, S_x^c(v'_{m,n})$$

In this expression certain derivatives of discrete model variables are found, namely $\Delta v'$ and $\Delta u''$. So, this cross-advective term uv_x has influences on the adjoint momentum equations which are solved in the first and second stages.

First, it contributes to the adjoint v momentum equation in the first stage corresponding to $\Delta v'_{m,n}$. Therefore, we have to examine the v momentum equations at the locations (m-2,n), (m-1,n), (m+1,n) and (m+2,n).

$$\begin{aligned}
\Delta v'_{m,n}\Bigg\{ &\cdots (\nu_v)''_{m-2,n}\left(\frac{\overline{\overline{u''}}_{m-2,n}}{12\Delta X}\right) + (\nu_v)''_{m-1,n}\left(\frac{4\overline{\overline{u''}}_{m-1,n}}{12\Delta X}\right) - \\
&(\nu_v)''_{m+1,n}\left(\frac{4\overline{\overline{u''}}_{m+1,n}}{12\Delta X}\right) - (\nu_v)''_{m+2,n}\left(\frac{\overline{\overline{u''}}_{m+2,n}}{12\Delta X}\right)\cdots\Bigg\}
\end{aligned} \tag{3.98}$$

Second, uv_x contributes to the adjoint u momentum equation in the second stage corresponding to $\Delta u_{m,n}$. Therefore, we have to examine the v momentum equations at the locations (m,n), (m+1,n), (m+1,n-1) and (m,n-1).

$$\Delta u_{m,n}\Big\{ \cdots (\nu_v)_{m,n}\frac{1}{4}S_x^c(\bar{v}'_{m,n}) + (\nu_v)_{m+1,n}\frac{1}{4}S_x^c(\bar{v}'_{m+1,n}) + (\nu_v)_{m+1,n-1}\frac{1}{4}S_x^c(\bar{v}'_{m+1,n-1}) + (\nu_v)_{m,n-1}\frac{1}{4}S_x^c(\bar{v}'_{m,n-1})\cdots \Big\} \tag{3.99}$$

Summary:

In summary the adjoint advective terms are (ignoring the boundary treatment and the degenerations caused by impeded points):

- In the adjoint u momentum equation associated with $\Delta u'_{m,n}$:

$$(\nu_u)'_{m,n}\frac{\left(u_{m+1,n}-u_{m-1,n}\right)}{2\Delta X}+(\nu_u)''_{m,n}\frac{\left(u''_{m+1,n}-u''_{m-1,n}\right)}{2\Delta X} \qquad (3.100)$$

Remark: the marked adjoint variables in these equations are the ones at the new time level.

- In the adjoint v momentum equation associated with $\Delta v'_{m,n}$:

$$\frac{v_{m,n-1}}{2\Delta Y}(\nu_v)'_{m,n-1}-\frac{v_{m,n+1}}{2\Delta Y}(\nu_v)'_{m,n+1}+\frac{\left(v''_{m,n-1}(\nu_v)''_{m,n-1}-v''_{m,n+1}(\nu_v)''_{m,n+1}\right)}{2\Delta Y} \qquad (3.101)$$

$$+(\nu_v)''_{m-2,n}\left(\frac{\overline{\overline{u''}}_{m-2,n}}{12\Delta X}\right)+(\nu_v)''_{m-1,n}\left(\frac{4\overline{\overline{u''}}_{m-1,n}}{12\Delta X}\right)-(\nu_v)''_{m+1,n}\left(\frac{4\overline{\overline{u''}}_{m+1,n}}{12\Delta X}\right)-(\nu_v)''_{m+2,n}\left(\frac{\overline{\overline{u''}}_{m+2,n}}{12\Delta X}\right) \qquad (3.102)$$

$$+(\nu_u)''_{m,n}\tfrac{1}{4}S^u_y(u''_{m,n})+(\nu_u)''_{m-1,n}\tfrac{1}{4}S^u_y(u''_{m-1,n})+(\nu_u)''_{m-1,n+1}\tfrac{1}{4}S^u_y(u''_{m-1,n+1})+(\nu_u)''_{m,n+1}\tfrac{1}{4}S^u_y(u''_{m,n+1}) \qquad (3.103)$$

$$+(\nu_u)'_{m,n}\tfrac{1}{4}S^c_y(u_{m,n})+(\nu_u)'_{m-1,n}\tfrac{1}{4}S^c_y(u_{m-1,n})+(\nu_u)'_{m-1,n+1}\tfrac{1}{4}S^c_y(u_{m-1,n+1})+(\nu_u)'_{m,n+1}\tfrac{1}{4}S^c_y(u_{m,n+1}) \qquad (3.104)$$

$$+(\nu_v)'_{m-2,n}\left(\frac{-\overline{\overline{u}}_{m-2,n}}{2\Delta X}\right)\quad \text{if } \overline{\overline{u}}_{m-2,n}\le 0 \qquad (3.105a)$$

$$+ \boxed{(\nu_v)'_{m-1,n}} \left(\frac{4\bar{\bar{u}}_{m-1,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m-1,n} \le 0 \qquad (3.105b)$$

$$+ \boxed{(\nu_v)'_{m,n}} \left(\frac{-3\bar{\bar{u}}_{m,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m,n} \le 0 ,$$

or

(3.105c)

$$+ \boxed{(\nu_v)'_{m,n}} \left(\frac{3\bar{\bar{u}}_{m,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m,n} > 0$$

$$+ \boxed{(\nu_v)'_{m+1,n}} \left(\frac{-4\bar{\bar{u}}_{m+1,n}}{2\Delta X} \right) \text{if } \bar{\bar{u}}_{m+1,n} > 0 \qquad (3.105d)$$

$$+ \boxed{(\nu_v)'_{m+2,n}} \left(\frac{\bar{\bar{u}}_{m+2,n}}{2\Delta X} \right) \quad \text{if } \bar{\bar{u}}_{m+2,n} > 0 \qquad (3.105e)$$

- In the adjoint v momentum equation associated with $\Delta v_{m,n}$:

$$(\nu_v)'_{m,n} \frac{\left(v_{m',n+1} - v_{m',n-1} \right)}{2\Delta Y} + \boxed{(\nu_v)_{m,n}} \frac{\left(\bar{v}'_{m,n+1} - \bar{v}'_{m,n-1} \right)}{2\Delta Y} \qquad (3.106)$$

- In the adjoint u momentum equation associated with $\Delta u_{m,n}$:

$$\frac{\left(U'_{m-1,n}(\nu_u)'_{m-1,n} - u'_{m+1,n}(\nu_u)'_{m+1,n} \right)}{2\Delta X} + \frac{\bar{u}'_{m-1,n}}{2\Delta X} \boxed{(\nu_u)_{m-1,n}} - \frac{\bar{u}'_{m+1,n}}{2\Delta X} \boxed{(\nu_u)_{m+1,n}} \qquad (3.107)$$

$$+ (\nu_u)'_{m,n-2} \left(\frac{\bar{\bar{v}}'_{m,n-2}}{12\Delta Y} \right) + (\nu_u)'_{m,n-1} \left(\frac{4\bar{\bar{v}}'_{m,n-1}}{12\Delta Y} \right) - (\nu_u)'_{m,n+1} \left(\frac{4\bar{\bar{v}}'_{m,n+1}}{12\Delta Y} \right) - (\nu_u)'_{m,n+2} \left(\frac{\bar{\bar{v}}'_{m,n+2}}{12\Delta Y} \right) \qquad (3.108)$$

$$+ (\nu_v)'_{m,n}\,\tfrac{1}{4}S^u_x(v'_{m,n}) + (\nu_v)'_{m+1,n}\,\tfrac{1}{4}S^u_x(v'_{m+1,n}) + (\nu_v)'_{m+1,n-1}\,\tfrac{1}{4}S^u_x(v'_{m+1,n-1}) + (\nu_v)'_{m,n-1}\,\tfrac{1}{4}S^u_x(v'_{m,n-1}) \quad (3.109)$$

$$+ (\nu_v)_{m,n}\,\tfrac{1}{4}S^c_x(\bar{v}'_{m,n}) + (\nu_v)_{m+1,n}\,\tfrac{1}{4}S^c_x(\bar{v}'_{m+1,n}) + (\nu_v)_{m+1,n-1}\,\tfrac{1}{4}S^c_x(\bar{v}'_{m+1,n-1}) + (\nu_v)_{m,n-1}\,\tfrac{1}{4}S^c_x(\bar{v}'_{m,n-1}) \quad (3.110)$$

$$+ (\nu_u)_{m,n+2}\left(\frac{\bar{v}'_{m,n+2}}{2\Delta Y}\right) \quad \text{if } \bar{v}'_{m,n+2} > 0 \quad (3.111a)$$

$$+ (\nu_u)_{m,n+1}\left(\frac{-4\bar{v}'_{m,n+1}}{2\Delta Y}\right) \text{if } \bar{v}'_{m,n+1} > 0 \quad (3.111b)$$

$$+ (\nu_u)_{m,n}\left(\frac{3\bar{v}'_{m,n}}{2\Delta Y}\right) \quad \text{if } \bar{v}'_{m,n} > 0\,,$$

or (3.111c)

$$+ (\nu_u)_{m,n}\left(\frac{-3\bar{v}'_{m,n}}{2\Delta Y}\right) \quad \text{if } \bar{v}'_{m,n} \le 0$$

$$+ (\nu_u)_{m,n-1}\left(\frac{4\bar{v}'_{m,n-1}}{2\Delta Y}\right) \text{if } \bar{v}'_{m,n-1} \le 0 \quad (3.111d)$$

$$+ (\nu_u)_{m,n-2}\left(\frac{-\bar{v}'_{m,n-2}}{2\Delta Y}\right) \text{if } \bar{v}'_{m,n-2} \le 0 \quad (3.111e)$$

Note that these two expressions are symmetrical with the adjoint advective terms in the first stage of the adjoint computation procedures. This is due to the ADI structure in WAQUA.

3.2.2.4. Curvilinear and spherical coordinates

In this subsection the advective terms for curvilinear and spherical coordinates are indicated. If the cross terms are ignored, the advective terms can be derived from the advective terms for WAQUA in rectangular coordinates. In this case it is only a matter of multiplying by coefficients. The structure of the equations remains the same.

For curvilinear models:

$$uu_{\xi} = \frac{u_{m,n}}{K^{u}_{m,n}} \frac{\left(u_{m+1,n} - u_{m-1,n} \right)}{2\Delta\xi} \tag{3.112}$$

$$vv_{\eta} = \frac{v_{m,n}}{E^{v}_{m,n}} \frac{\left(v_{m,n+1} - v_{m,n-1} \right)}{2\Delta\eta} \tag{3.113}$$

The second order difference operators:

$$S^{c}_{\eta}(u_{m,n}) = \frac{1}{E_{m,n}} \left\{ \frac{\frac{2}{3}\left(u_{m,n+1} - u_{m,n-1} \right)}{2\Delta\eta} + \frac{\frac{1}{3}\left(u_{m,n+2} - u_{m,n-2} \right)}{4\Delta\eta} \right\} \tag{3.114}$$

$$S^{u}_{\eta}(u_{m,n}) = \frac{1}{E_{m,n}} \begin{cases} \dfrac{\left(\frac{3}{2} u_{m,n} - 2u_{m,n-1} + \frac{1}{2} u_{m,n-2} \right)}{\Delta\eta} & , \text{ if } \bar{\bar{v}}_{m,n} > 0 \\ \dfrac{\left(-\frac{3}{2} u_{m,n} + 2u_{m,n+1} - \frac{1}{2} u_{m,n+2} \right)}{\Delta\eta} & , \text{ if } \bar{\bar{v}}_{m,n} \le 0 \end{cases} \tag{3.115}$$

$$S^{c}_{\xi}(v_{m,n}) = \frac{1}{K_{m,n}} \left\{ \frac{\frac{2}{3}\left(v_{m+1,n} - v_{m-1,n} \right)}{2\Delta\xi} + \frac{\frac{1}{3}\left(v_{m+2,n} - v_{m-2,n} \right)}{4\Delta\xi} \right\} \tag{3.116}$$

$$S^{u}_{\xi}(v_{m,n}) = \frac{1}{K_{m,n}} \begin{cases} \dfrac{\left(\frac{3}{2} v_{m,n} - 2v_{m-1,n} + \frac{1}{2} v_{m-2,n} \right)}{\Delta\xi} & , \text{ if } \bar{\bar{u}}_{m,n} > 0 \\ \dfrac{\left(-\frac{3}{2} v_{m,n} + 2v_{m+1,n} - \frac{1}{2} v_{m+2,n} \right)}{\Delta\xi} & , \text{ if } \bar{\bar{u}}_{m,n} \le 0 \end{cases} \tag{3.117}$$

At source code level there is no difference between WAQUA in curvilinear or spherical coordinates. Everything is fixed by the choice of the variables $K_{m,n}$ and $E_{m,n}$, the distances between depth points in the ξ and η directions, see subsection 3.2.1.

From this, together with the mathematical derivation in the previous chapters, it follows that the adjoint advective terms for curvilinear models and models with spherical coordinates are (compare with equations (3.100) to (3.111)):

- In the adjoint u momentum equation associated with $\Delta u'_{m,n}$

$$(\nu_u)'_{m,n}\frac{(u_{m+1,n}-u_{m-1,n})}{K^u_{m,n}\ 2\Delta\xi}+(\nu_u)''_{m,n}\frac{(u''_{m+1,n}-u''_{m-1,n})}{K^u_{m,n}\ 2\Delta\xi} \quad (3.118)$$

- In the adjoint v momentum equation associated with $\Delta v'_{m,n}$

$$\frac{v_{m,n-1}}{E^v_{m,n-1}\ 2\Delta\eta}(\nu_v)'_{m,n-1}-\frac{v_{m,n+1}}{E^v_{m,n+1}\ 2\Delta\eta}(\nu_v)'_{m,n+1}$$
$$+\left(\frac{v''_{m,n-1}(\nu_v)''_{m,n-1}}{E^v_{m,n-1}\ 2\Delta\eta}-\frac{v''_{m,n+1}(\nu_v)''_{m,n+1}}{E^v_{m,n+1}\ 2\Delta\eta}\right) \quad (3.119)$$

$$+\frac{(\nu_v)''_{m-2,n}}{K_{m-2,n}}\left(\frac{\overline{\overline{u''}}_{m-2,n}}{12\Delta\xi}\right)+\frac{(\nu_v)''_{m-1,n}}{K_{m-1,n}}\left(\frac{4\overline{\overline{u''}}_{m-1,n}}{12\Delta\xi}\right)-$$
$$\frac{(\nu_v)''_{m+1,n}}{K_{m+1,n}}\left(\frac{4\overline{\overline{u''}}_{m+1,n}}{12\Delta\xi}\right)-\frac{(\nu_v)''_{m+2,n}}{K_{m+2,n}}\left(\frac{\overline{\overline{u''}}_{m+2,n}}{12\Delta\xi}\right) \quad (3.120)$$

$$+(\nu_u)''_{m,n}\tfrac{1}{4}S^u_y(u''_{m,n})+(\nu_u)''_{m-1,n}\tfrac{1}{4}S^u_y(u''_{m-1,n})+$$
$$(\nu_u)''_{m-1,n+1}\tfrac{1}{4}S^u_y(u''_{m-1,n+1})+(\nu_u)''_{m,n+1}\tfrac{1}{4}S^u_y(u''_{m,n+1}) \quad (3.121)$$

$$+(\nu_u)'_{m,n}\tfrac{1}{4}S^c_y(u_{m,n})+(\nu_u)'_{m-1,n}\tfrac{1}{4}S^c_y(u_{m-1,n})+$$
$$(\nu_u)'_{m-1,n+1}\tfrac{1}{4}S^c_y(u_{m-1,n+1})+(\nu_u)'_{m,n}\tfrac{1}{4}S^c_y(u_{m,n+1}) \quad (3.122)$$

$$+(\nu_v)'_{m-2,n}\left(\frac{-\bar{u}_{m-2,n}}{K_{m-2,n}\ 2\Delta\xi}\right)\quad \text{if } \bar{u}_{m-2,n}\le 0 \quad (3.123a)$$

$$+(\nu_v)'_{m-1,n}\left(\frac{4\bar{u}_{m-1,n}}{K_{m-1,n}\ 2\Delta\xi}\right)\quad \text{if } \bar{u}_{m-1,n}\le 0 \quad (3.123b)$$

$$+(\nu_v)'_{m,n}\left(\frac{-3\bar{u}_{m,n}}{K_{m,n}\ 2\Delta\xi}\right)\quad \text{if } \bar{u}_{m,n}\le 0\,,$$

or (3.123c)

$$+ \boxed{(\nu_v)'_{m,n}} \left(\frac{3\bar{\bar{u}}_{m,n}}{K_{m,n}\ 2\Delta\xi} \right) \quad \text{if } \bar{\bar{u}}_{m,n} > 0$$

$$+ \boxed{(\nu_v)'_{m+1,n}} \left(\frac{-4\bar{\bar{u}}_{m+1,n}}{K_{m+1,n}\ 2\Delta\xi} \right) \text{ if } \bar{\bar{u}}_{m+1,n} > 0 \qquad (3.123d)$$

$$+ \boxed{(\nu_v)'_{m+2,n}} \left(\frac{\bar{\bar{u}}_{m+2,n}}{K_{m+2,n}\ 2\Delta\xi} \right) \text{ if } \bar{\bar{u}}_{m+2,n} > 0 \qquad (3.123e)$$

- In the adjoint v momentum equation associated with $\Delta v_{m,n}$

$$(\nu_v)'_{m,n} \frac{\left(v'_{m,n+1} - v'_{m,n-1} \right)}{E^v_{m,n}\ 2\Delta\eta} + \boxed{(\nu_v)_{m,n}} \frac{\left(\bar{v}'_{m,n+1} - \bar{v}'_{m,n-1} \right)}{E^v_{m,n}\ 2\Delta\eta} \qquad (3.124)$$

- In the adjoint u momentum equation associated with $\Delta u_{m,n}$

$$\left(\frac{u'_{m-1,n}\,(\nu_u)'_{m-1,n}}{K^u_{m-1,n}\ 2\Delta\xi} - \frac{u'_{m+1,n}(\nu_u)'_{m+1,n}}{K^u_{m+1,n}\ 2\Delta\xi} \right) + \frac{\bar{u}'_{m-1,n}}{K^u_{m-1,n}\ 2\Delta\xi} \boxed{(\nu_u)_{m-1,n}} - \frac{\bar{u}'_{m+1,n}}{K^u_{m+1,n}\ 2\Delta\xi} \boxed{(\nu_u)_{m+1,n}} \qquad (3.125)$$

$$+ \frac{(\nu_u)'_{m,n-2}}{E_{m,n-2}} \left(\frac{\bar{\bar{v}}'_{m,n-2}}{12\Delta\eta} \right) + \frac{(\nu_u)'_{m,n-1}}{E_{m,n-1}} \left(\frac{4\bar{\bar{v}}'_{m,n-1}}{12\Delta\eta} \right) - \frac{(\nu_u)'_{m,n+1}}{E_{m,n+1}} \left(\frac{4\bar{\bar{v}}'_{m,n+1}}{12\Delta\eta} \right) - \frac{(\nu_u)'_{m,n+2}}{E_{m,n+2}} \left(\frac{\bar{\bar{v}}'_{m,n+2}}{12\Delta\eta} \right) \qquad (3.126)$$

$$+ (\nu_v)'_{m,n}\ \tfrac{1}{4} S^u_x(v'_{m,n}) + (\nu_v)'_{m+1,n}\ \tfrac{1}{4} S^u_x(v'_{m+1,n}) + (\nu_v)'_{m+1,n-1}\ \tfrac{1}{4} S^u_x(v'_{m+1,n-1}) + (\nu_v)'_{m,n-1}\ \tfrac{1}{4} S^u_x(v'_{m,n-1}) \qquad (3.127)$$

$$+ (\nu_v)_{m,n}\tfrac{1}{4}S_x^c(\bar{v}'_{m,n}) + (\nu_v)_{m+1,n}\tfrac{1}{4}S_x^c(\bar{v}'_{m+1,n}) + (\nu_v)_{m+1,n-1}\tfrac{1}{4}S_x^c(\bar{v}'_{m+1,n-1}) + (\nu_v)_{m,n-1}\tfrac{1}{4}S_x^c(\bar{v}'_{m,n-1}) \quad (3.128)$$

$$+ (\nu_u)_{m,n+2}\left(\frac{\bar{v}'_{m,n+2}}{E_{m,n+2}\,2\Delta\eta}\right) \text{ if } \bar{v}'_{m,n+2} > 0 \quad (3.129a)$$

$$+ (\nu_u)_{m,n+1}\left(\frac{-4\bar{v}'_{m,n+1}}{E_{m,n+1}\,2\Delta\eta}\right) \text{ if } \bar{v}'_{m,n+1} > 0 \quad (3.129b)$$

$$+ (\nu_u)_{m,n}\left(\frac{3\bar{v}'_{m,n}}{E_{m,n}\,2\Delta\eta}\right) \text{ if } \bar{v}'_{m,n} > 0\,,$$

or

(3.129c)

$$+ (\nu_u)_{m,n}\left(\frac{-3\bar{v}'_{m,n}}{E_{m,n}\,2\Delta\eta}\right) \text{ if } \bar{v}'_{m,n} \le 0$$

$$+ (\nu_u)_{m,n-1}\left(\frac{4\bar{v}'_{m,n-1}}{E_{m,n-1}\,2\Delta\eta}\right) \text{ if } \bar{v}'_{m,n-1} \le 0 \quad (3.129d)$$

$$+ (\nu_u)_{m,n-2}\left(\frac{-\bar{v}'_{m,n-2}}{E_{m,n-2}\,2\Delta\eta}\right) \text{ if } \bar{v}'_{m,n-2} \le 0 \quad (3.129e)$$

Remark: The boundary treatment and the degenerations caused by impeded points are ignored in this subsection. See appendix A for more information on this subject.

3.2.3. Boundary conditions

In this subsection the adjoint boundary conditions are deduced. It is only necessary to solve these adjoint boundary conditions is only necessary when estimating uncertain parameters in the WAQUA boundary conditions. We will begin by describing the WAQUA boundary conditions.

In order to obtain a unique solution to the WAQUA model equations (3.1-3.3) a set of boundary conditions is prescribed. Two types of boundaries are considered: open and closed. At closed boundaries such as coastlines and dams the boundary condition yields:

$$v_{\perp} = 0$$

This means that no inflow or outflow can occur through these boundaries. Open boundaries are non physical (mathematical) boundaries that are to delimit the domain of the model. In the case of open boundaries two boundary conditions are required. In WAQUA the first requirement is fulfilled by placing velocity blockades at the open boundary. This guarantees that the velocity parallel to the boundary has a zero value. The second requirement is satisfied by imposing a water level boundary condition in an explicit way. This boundary condition consists of a series of cosines of harmonic constituents:

$$\zeta(t) = \zeta_0 + \sum_{i=1}^{n} A_i \cos(\omega_i t - \phi_i) \qquad (3.130)$$

in which:

$\zeta(t)$	=	water level elevation at time t
ζ_0	=	averaged sea surface
n	=	number of harmonic constituents
A_i	=	amplitude of harmonic constituent i
ω_i	=	angular velocity of harmonic constituent i
ϕ_i	=	phase of harmonic constituent i

The discretized equation in space and time for the boundary condition described by (3.130) is the starting point for the deduction of the corresponding adjoint boundary conditions. Similar to the derivation of the adjoint model equations, the adjoint boundary conditions can be derived by following the next three steps:

- The boundary conditions described above are constraints just like the WAQUA model equations.

  Remark: Since the boundary conditions are not defined by state variables at interior points of the model and since it is solely a function of model parameters, the deduction of the adjoint model equations in the previous section does not change. However, some terms concerning the adjoint variables at the boundary must be added.

- The terms to be added are derived from the linearized WAQUA equations by looking to see which terms contribute to the boundary.

- The adjoint boundary conditions are then deduced by rearranging the contributing terms and assigning them a value in such a way that all $\Delta\zeta$ do not contribute to the expression of the gradient.

In the next part of this subsection the three steps are performed for each open boundary in order to derive the corresponding adjoint boundary conditions.

Left-hand open boundary:

The velocity parallel to the boundary equals zero. Therefore, the v momentum equation does not contribute to the boundary. The continuity equation and the u momentum equation do contribute. Consider point (m,n) to be on the boundary. The contributions to the boundary are as follows:

- Adjoint equation for $\Delta\zeta'_{m,n}$:

  Contribution of the continuity equation in the first stage (from $t \rightarrow t+½\Delta t$) in (m+1,n):

$$\frac{(\nu_\zeta)'_{m+1,n}}{K^{\eta}_{m+1,n} E^{\xi}_{m+1,n}} \left[\frac{-\frac{1}{2} u'_{m,n} E_{m,n}}{\Delta\xi} \right]$$

  Contribution of the u momentum equation in the first stage in (m,n):

$$(\nu_u)'_{m,n} \left[\frac{-g}{K^{u}_{m,n} \Delta\xi} + \frac{1}{2} fruw\, l'_{m,n} \right]$$

  Contribution of the u momentum equation in the second stage (from $t+½\Delta t$ $t+\Delta t$) in (m,n):

$$(\nu_u)''_{m,n} \left[\frac{-g}{K^{u}_{m,n} \Delta\xi} + \frac{1}{2} fruw\, l'_{m,n} \right]$$

  Contribution of the continuity equation at the second stage in (m+1,n):

$$\frac{(\nu_\zeta)''_{m+1,n}}{K^{\eta}_{m+1,n} E^{\xi}_{m+1,n}} \left[\frac{-\frac{1}{2} u'_{m,n} E_{m,n}}{\Delta\xi} \right]$$

Contribution of the WAQUA boundary condition:

$$(\nu_\zeta)'_{m,n}$$

By adding these contributions, including the contribution of the WAQUA boundary condition, and rearranging the variables, the adjoint boundary condition is derived:

$$(\nu_\zeta)'_{m,n} = \left(\frac{g}{K^u_{m,n}\,\Delta\xi} - \frac{1}{2}\text{fruw}\,l'_{m,n}\right)\left[(\nu_u)'_{m,n} + (\nu_u)''_{m,n}\right] + \frac{\frac{1}{2}u'_{m,n}\,E_{m,n}}{\Delta\xi}\left[\frac{(\nu_\zeta)'_{m+1,n} + (\nu_\zeta)''_{m+1,n}}{K^\eta_{m+1,n}E^\xi_{m+1,n}}\right]$$

- Adjoint equation for $\Delta\zeta_{m,n}$:

$$(\nu_\zeta)_{m,n} = 0$$

Right-hand open boundary:

As for the left-hand open boundary the v momentum equation does not contribute to the boundary. The continuity equation and the u momentum equation do. Consider point (m,n) to be on the boundary. The contributions to the boundary are as follows:

Adjoint equation for $\Delta\zeta'_{m,n}$:

Contribution of the continuity equation in the first stage (from t $\rightarrow$ t+½Δt) in (m-1,n):

$$\frac{(\nu_\zeta)'_{m-1,n}}{K^{\eta}_{m-1,n}E^{\xi}_{m-1,n}}\left[\frac{\frac{1}{2}u'_{m-1,n}E_{m-1,n}}{\Delta\xi}\right]$$

Contribution of the u momentum equation in the first stage in (m-1,n):

$$(\nu_u)'_{m-1,n}\left[\frac{g}{K^{u}_{m-1,n}\Delta\xi}+\frac{1}{2}\text{fruw}\,l'_{m-1,n}\right]$$

Contribution of the u momentum equation in the second stage (from t+½Δt t+Δt) in (m-1,n):

$$(\nu_u)''_{m-1,n}\left[\frac{g}{K^{u}_{m-1,n}\Delta\xi}+\frac{1}{2}\text{fruw}\,l'_{m-1,n}\right]$$

Contribution of the continuity equation in the second stage in (m-1,n):

$$\frac{(\nu_\zeta)''_{m-1,n}}{K^{\eta}_{m-1,n}E^{\xi}_{m-1,n}}\left[\frac{\frac{1}{2}u'_{m-1,n}E_{m-1,n}}{\Delta\xi}\right]$$

Contribution of the WAQUA boundary condition:

$$(\nu_\zeta)'_{m,n}$$

By adding the contributions and rearranging the variables, the adjoint boundary condition yields:

$$(\nu_\zeta)'_{m,n} = -\left(\frac{g}{K^{u}_{m-1,n}\Delta\xi}+\frac{1}{2}\text{fruw}\,l'_{m-1,n}\right)\left[(\nu_u)'_{m-1,n}+(\nu_u)''_{m-1,n}\right] + \frac{-\frac{1}{2}u'_{m-1,n}E_{m-1,n}}{\Delta\xi}\left[\frac{(\nu_\zeta)'_{m-1,n}+(\nu_\zeta)''_{m-1,n}}{K^{\eta}_{m-1,n}E^{\xi}_{m-1,n}}\right]$$

- Adjoint equation for $\Delta\zeta_{m,n}$:

  $(\nu_\zeta)_{m,n} = 0$

Upper open boundary:

The velocity parallel to the boundary equals zero. Therefore, the u momentum equation does not contribute to the boundary. The continuity equation and the v momentum equation do contribute. Consider point (m,n) to be on the boundary. The contributions to the boundary are as follows:

- Adjoint equation for $\Delta\zeta'_{m,n}$:

  $(\nu_\zeta)'_{m,n} = 0$

- Adjoint equation for $\Delta\zeta_{m,n}$:

  Contribution of the continuity equation in the second stage (from t-½Δt $\rightarrow$ t) in (m,n-1):

$$\frac{(\nu_\zeta)_{m,n-1}}{K^\eta_{m,n-1}E^\xi_{m,n-1}}\left[\frac{\frac{1}{2}v_{m,n-1}K_{m,n-1}}{\Delta\eta}\right]$$

  Contribution of the v momentum equation in the second stage in (m,n-1):

$$(\nu_v)_{m,n-1}\left[\frac{g}{E^v_{m,n-1}\Delta\eta}+\frac{1}{2}\text{frvwl}_{m,n-1}\right]$$

  Contribution of the v momentum equation in the first stage (from t $\rightarrow$ t+½Δt) in (m,n-1):

$$(\nu_v)'_{m,n-1}\left[\frac{g}{E^v_{m,n-1}\Delta\eta}+\frac{1}{2}\text{frvwl}_{m,n-1}\right]$$

  Contribution of the continuity equation in the first stage in (m,n-1):

$$\frac{(\nu_\zeta)'_{m,n-1}}{K^\eta_{m,n-1}E^\xi_{m,n-1}}\left[\frac{\frac{1}{2}v_{m,n-1}K_{m,n-1}}{\Delta\eta}\right]$$

  Contribution of the WAQUA boundary condition:

$(\nu_\zeta)_{m,n}$

By adding the contributions and rearranging the variables, the adjoint boundary condition is described by:

$$(\nu_\zeta)_{m,n} = -\left(\frac{g}{E^v_{m,n-1}\Delta\eta} + \frac{1}{2}frvwl_{m,n-1}\right)\left[(\nu_v)_{m,n-1} + (\nu_v)'_{m,n-1}\right] + \frac{-\frac{1}{2}v_{m,n-1}K_{m,n-1}}{\Delta\eta}\left[\frac{(\nu_\zeta)_{m,n-1} + (\nu_\zeta)'_{m,n-1}}{K^\eta_{m,n-1}E^\xi_{m,n-1}}\right]$$

Lower open boundary:

As for the upper open boundary the u momentum equation does not contribute to the boundary. The continuity equation and the v momentum equation do. Consider point (m,n) to be on the boundary. The contributions to the boundary are as follows:

- Adjoint equation for $\Delta\zeta'_{m,n}$:

  $(\nu_\zeta)'_{m,n} = 0$

- Adjoint equation for $\Delta\zeta_{m,n}$:

  Contribution of the continuity equation in the second stage (from t-½Δt → t) in (m,n+1):

$$\frac{(\nu_\zeta)_{m,n+1}}{K^\eta_{m,n+1}E^\xi_{m,n+1}}\left[\frac{-\frac{1}{2}v_{m,n}K_{m,n}}{\Delta\eta}\right]$$

  Contribution of the v momentum equation in the second stage in (m,n):

$$(\nu_v)_{m,n}\left[\frac{-g}{E^v_{m,n}\Delta\eta} + \frac{1}{2}frvwl_{m,n}\right]$$

  Contribution of the v momentum equation in the first stage (from t → t+½Δt) in (m,n):

$$(\nu_v)'_{m,n}\left[\frac{-g}{E^v_{m,n}\Delta\eta} + \frac{1}{2}frvwl_{m,n}\right]$$

  Contribution of the continuity equation in the first stage in

m,n+1):

$$\frac{(\nu_\zeta)'_{m,n+1}}{K^{\eta}_{m,n+1}E^{\xi}_{m,n+1}}\left[\frac{-\frac{1}{2}v_{m,n}K_{m,n}}{\Delta\eta}\right]$$

Contribution of the WAQUA boundary condition:

$$(\nu_\zeta)_{m,n}$$

By adding the contributions and rearranging the variables, the adjoint boundary condition is described by:

$$(\nu_\zeta)_{m,n} = \left(\frac{g}{E^{v}_{m,n}\Delta\eta} - \frac{1}{2}frvwl_{m,n}\right)\left[(\nu_v)_{m,n} + (\nu_v)'_{m,n}\right] + \frac{\frac{1}{2}v_{m,n}K_{m,n}}{\Delta\eta}\left[\frac{(\nu_\zeta)_{m,n+1} + (\nu_\zeta)'_{m,n+1}}{K^{\eta}_{m,n+1}E^{\xi}_{m,n+1}}\right]$$

Diagonal open boundary:

Some models have an open boundary which is diagonal. In this case the boundary condition is a combination of two boundary conditions. For example in the case of the Continental Shelf Model the boundary condition is a combination of the left-hand and upper boundary conditions. In this case the boundary condition becomes:

$$(\nu_\zeta)'_{m,n} = \left(\frac{g}{K^{u}_{m,n}\Delta\xi} - \frac{1}{2}fruwl'_{m,n}\right)\left[(\nu_u)'_{m,n} + (\nu_u)''_{m,n}\right] + \frac{\frac{1}{2}u'_{m,n}E_{m,n}}{\Delta\xi}\left[\frac{(\nu_\zeta)'_{m+1,n} + (\nu_\zeta)''_{m+1,n}}{K^{\eta}_{m+1,n}E^{\xi}_{m+1,n}}\right]$$

$$(\nu_\zeta)_{m,n} = -\left(\frac{g}{E^{v}_{m,n-1}\Delta\eta} + \frac{1}{2}frvwl_{m,n-1}\right)\left[(\nu_v)_{m,n-1} + (\nu_v)'_{m,n-1}\right] + \frac{-\frac{1}{2}v_{m,n-1}K_{m,n-1}}{\Delta\eta}\left[\frac{(\nu_\zeta)_{m,n-1} + (\nu_\zeta)'_{m,n-1}}{K^{\eta}_{m,n-1}E^{\xi}_{m,n-1}}\right]$$

Remarks:

- Only if uncertain parameters of the WAQUA boundary conditions are estimated is it necessary to calculate the corresponding adjoint variables at the boundary.
- The adjoint boundary conditions are solved after solving the adjoint model equations. This is allowed, since the

boundary condition is not defined by state variables at interior points of the model and since it is solely a function of model parameters.

3.2.4. Dryfall

In this subsection the drying and flooding procedures in WAQUA are described first. Then the adjoint drying and flooding procedures are derived. For more information on drying and flooding during tidal computations, see [Mouthaan, 1992] and [Stelling, 1986].

Drying and flooding procedures in WAQUA

WAQUA probably does not calculate the water flow very accurately in parts of estuaries with a very low water level. Drying procedures have been developed to prevent calculations with physically unrealistic values. Several procedures for drying and flooding of tidal flats are applied in WAQUA in order to solve the shallow water equations correctly. These procedures decide which grid points are included in the next calculation. The decisions are made on the basis of the calculated water level elevations. The criterion is the local water depth. Several definitions of the local water depth are possible in the case of a water level point. In the case of a velocity point there is only one definition.

Checks of local water depths at velocity points are always performed in the calculation. Th local waterdepth must be positive, as otherwise the continuity equation and the momentum equations will not be solved correctly. In addition, it is also possible to check local water depths at water level points. This is important, especially in the case of transport simulations.

The drying and flooding procedures is described below. The procedures are described for the 'U part' of the ADI method, applied to the interior points of the model.

At the beginning of the first stage of the ADI method in the u direction, first the local water depth is calculated at every velocity point $u_{m,n}$. The local waterdepth in a u velocity point is defined by:

$$\tfrac{1}{2}[\ \zeta_{m,n} + \zeta_{m+1,n} + d_{m,n} + d_{m,n-1}\ ]$$

- The flooding procedure
  If the local waterdepth exceeds the threshold value VAR (which is given in the WAQUA user input) and if velocity point $u_{m,n}$ was not included in the calculation for the

previous time step because of dryfall, that velocity point will now be involved in the calculation.

After this check the continuity equation and the u momentum equation are solved for this row. After this row has been completed the drying procedure at velocity points is activated.

In this first stage of the ADI method in the u direction the drying procedure only checks the u velocity points. In addition it is possible to active drying procedures that check water level points.

- The drying procedure in velocity point $u_{m,n}$
  If the local water depth at the velocity point is less than ½ VAR the point $u_{m,n}$ is no longer involved in the calculation. The dryfall threshold is half the flooding threshold. This prevents points from becoming active for one time step and inactive again for the next.

- Optional drying procedures at water level point $\zeta_{m,n}$
  In WAQUA the user has three options for defining local water depths at water level points. The user also has the option to skip this procedure. The definitions of the local water depths in water level points are:

  1) maximum criterion:

     $$\zeta_{m,n} + \tfrac{1}{2} * [\, \max(d_{m,n}, d_{m-1,n-1}) + \max(d_{m-1,n}, d_{m,n-1}) \,]$$

  2) averaged criterion:

     $$\zeta_{m,n} + \tfrac{1}{4} * [\, d_{m,n} + d_{m-1,n-1} + d_{m-1,n} + d_{m,n-1} \,]$$

  3) minimum criterion:

     $$\zeta_{m,n} + \tfrac{1}{2} * [\, \min(d_{m,n}, d_{m-1,n-1}) + \min(d_{m-1,n}, d_{m,n-1}) \,]$$

  4) no check at water level points

If the user chooses one of the first three options and if the corresponding local water depth at the water level point is less than ½ VAR, the two adjacent velocity points $u_{m,n}$ en $u_{m-1,n}$ are no longer involved in the calculation. If one or more points fall dry, the continuity equation and the u momentum equation are solved again for this row, with these velocity points as stationary points. This means that during this step these velocity points are considered to be closed boundary points. Normally the new velocities are calculated by means of the momentum equations. In the case of dryfall a velocity blockade is placed in order to give the new velocity a zero value.

Before calculating the second stage of the ADI method in u direction, the u velocity points are checked for dryfall. This drying procedure has already been checked during the calculation process, though. Next, the new u velocities are calculated according to the previous state variables. After this the drying procedures do not check the u velocity points any more, since the new water level elevations have not yet been calculated.

All these procedures have one thing in common: the decision about which points should be involved in the next calculation step is made on the basis of the water depths. If points are excluded, the velocity points are made stagnant. These velocity points are regarded by WAQUA as closed boundary points with zero values. If they are re-incorporated in the calculation, they are no longer considered to be closed boundary points. The alternating drying and flooding of the tidal flats means that moving closed boundaries can be created in WAQUA.

The adjoint drying and flooding procedures

The dynamic WAQUA equations are important for deriving the adjoint equations. The starting point for deducing the adjoint variables is the way that WAQUA calculates new state variables at a certain point of time. If drying occurs in WAQUA, the adjoint equations at the corresponding time steps must be modified. The whole process of drying and flooding in WAQUA can be reduced to the following essential property: either the velocities are calculated by the normal momentum equations, or they are determined by imposing zero values. As a consequence of this the exact formulations of the different drying and flooding procedures are not important to WAQAD. Only the time steps during which velocities points are treated as closed boundary conditions are important. A universal adjoint drying and flooding procedure can be based on this characteristic.

The adjoint equations derived without the drying and flooding procedure are the starting point of the next analysis. Suppose that at the first stage (from $t \rightarrow t+½\Delta t$) velocity point $u_{m,n}$ is no longer involved in the WAQUA calculation due to an drying procedure (which may be arbitrary). The following can be derived:

- $u'_{m,n} = 0.$ instead of being calculated by the u momentum equation.

- The equation $u'_{m,n} = 0.$ does not explicitly contain any unknown model parameter. The contribution to the calculation of the gradient is therefore equal to zero, irrespective of the fact that this constraint is modelled as a known or unknown boundary condition in the reverse calculation process.

- $(\nu_u)'_{m,n}$ disappears from all the adjoint equations, therefore $(\nu_u)'_{m,n}$ has a zero value in all these equations.

The universal adjoint drying procedure is therefore similar to the WAQUA drying procedure:

$(\nu_u)'_{m,n} = 0$ instead of being calculated by the adjoint u momentum equation.

The preceding reasoning is in fact the adjoint approach for velocity boundaries in WAQUA, that is, boundary conditions in WAQUA correspond with homogeneous boundary conditions in WAQAD. In this situation WAQUA state variables at boundary points are also determined by assigning the variable a certain value instead of solving the momentum equation, or instead of solving the continuity equation in the case of a water level boundary condition. Terms with state variables at interior points do not appear in the linearizations of the WAQUA boundary conditions. In principle, adjoint boundary variables do not appear in the adjoint model equations for the interior state variables either. This is equivalent to solving the adjoint model equations with homogeneous WAQAD boundary conditions. Only when parameters in the WAQUA boundary conditions are estimated is it necessary to determine the contribution to the gradient for the adjoint state variables at the boundary. This can be interpreted as a WAQAD boundary condition. The WAQAD boundary conditions are solved after solving the adjoint model equations for the interior state variables.

Drying and flooding of tidal flats in WAQUA can be interpreted as the movement of the closed boundary conditions. This is expressed in WAQAD by the movement of the corresponding homogeneous boundary conditions.

Finally, it must be remembered that the adjoint equations are solved backwards in time when implementing the adjoint drying and flooding procedures. The values of the WAQUA state variables are therefore known at every time step. To discover the times of drying in WAQUA it is not necessary to check the local water depths with the drying criteria described. A simple test to check if the velocity at a certain point of time is exactly equal to zero will be sufficient.

3.3. The adjoint solver

This section deals with the method for solving the deduced adjoint equations for the two- dimensional shallow water flow model. The method for solving the adjoint equations also has a two- stage time-splitting structure.

In subsection 3.3.1 the method for solving the adjoint equations without advective terms is described. Subsection 3.3.2 gives the modifications to solving the adjoint equations when advective terms are included. Subsection 3.3.3 gives an overview of solving the adjoint model equations in the case of dryfall.

3.3.1. Method for solving the adjoint model equations

The adjoint model equations are solved in the reversed order compared with WAQUA. In the first stage in WAQUA the v momentum equation is solved in module VYD first and then the continuity equation and the u momentum equation are solved in module SUV. In the first stage in WAQAD the adjoint continuity equation and the adjoint u momentum equation are solved in module AD-SUV first and then the adjoint v momentum equation is solved in module AD-VYD. In the second stage in WAQUA the u momentum equation is solved in module UXD first and then the continuity equation and the v momentum equation are solved in module SVU. In the second stage in WAQAD the adjoint continuity equation and the adjoint v momentum equation are solved in module AD-SUV first and then the adjoint u momentum equation is solved in module AD-UXD. An overview of the WAQUA and WAQAD computation procedures is given below:

The WAQUA procedures:

VYD computes v'
SUV computes ζ', u'
UXD computes u''
SVU computes ζ'', v''

The WAQAD procedures:

AD-SUV computes $(\nu_\zeta)', (\nu_u)'$ to make $\Delta\zeta', \Delta u'$ vanish
AD-VYD computes $(\nu_v)'$ to make $\Delta v'$ vanish
AD-SVU computes $(\nu_\zeta), (\nu_v)$ to make $\Delta\zeta, \Delta v$ vanish
AD-UXD computes (ν_u) to make Δu vanish

In the next part of this subsection the solution method in the WAQAD modules AD-SUV, AD-VYD, AD-SVU and AD-UXD is described.

AD-SUV

The adjoint u momentum equation and the adjoint continuity equation in the first stage, from $t+\Delta t \rightarrow t+½\Delta t$, are implicitly coupled equations.

The adjoint u velocity at time $t+½\Delta t$ is expressed as a function of the unknown adjoint water levels at time $t+½\Delta t$:

$$(\nu_u)'_{m,n} = DD_{m+1} - CC_{m+1}\left[\frac{(\nu_\zeta)'_{m+1,n}}{K^\eta_{m+1,n}E^\xi_{m+1,n}} - \frac{(\nu_\zeta)'_{m,n}}{K^\eta_{m,n}E^\xi_{m,n}}\right]$$

The coefficients CC_{m+1} and DD_{m+1} are determined by:

$$CC_{m+1} = -\frac{(H^u)'_{m,n}E_{m,n}}{\Delta\xi[\frac{1}{½\Delta t} + fruu'_{m,n}]}$$

$$DD_{m+1} = \frac{[\frac{1}{½\Delta t} - fruu'_{m,n}](\nu_u)''_{m,n}}{\frac{1}{½\Delta t} + fruu'_{m,n}} - \frac{(H^u)'_{m,n}E_{m,n}}{\Delta\xi[\frac{1}{½\Delta t} + fruu'_{m,n}]}\left[\frac{(\nu_\zeta)''_{m,n}}{K^\eta_{m,n}E^\xi_{m,n}} - \frac{(\nu_\zeta)''_{m+1,n}}{K^\eta_{m+1,n}E^\xi_{m+1,n}}\right]$$

The adjoint u velocity at time $t+½\Delta t$ is eliminated from the adjoint continuity equation. This results in a tridiagonal system of unknown adjoint water levels at time $t+½\Delta t$ for each row:

$$A_m(\nu_\zeta)'_{m-1,n} + B_m(\nu_\zeta)'_{m,n} + C_m(\nu_\zeta)'_{m+1,n} = D_m$$

Coefficients A_m, B_m, C_m and D_m are calculated by:

$$A_m = \frac{1}{K^\eta_{m-1,n}E^\xi_{m-1,n}}\left\{[\frac{g}{K^u_{m-1,n}\Delta\xi} + \frac{1}{2}fruwl'_{m-1,n}]CC_m + \frac{\frac{1}{2}u'_{m-1,n}E_{m-1,n}}{\Delta\xi}\right\}$$

$$B_m = \frac{1}{K^{\eta}_{m,n} E^{\xi}_{m,n}} \left\{ \left[\frac{1}{2} fruw\, l'_{m,n} - \frac{g}{K^{u}_{m,n} \Delta\xi} \right] CC_{m+1} - \left[\frac{g}{K^{u}_{m-1,n} \Delta\xi} + \frac{1}{2} fruw\, l'_{m-1,n} \right] CC_m + \frac{\frac{1}{2}\left[u'_{m,n} E_{m,n} - u'_{m-1,n} E_{m-1,n} \right]}{\Delta\xi} \right\} + \frac{1}{\frac{1}{2}\Delta t}$$

$$C_m = \frac{1}{K^{\eta}_{m+1,n} E^{\xi}_{m+1,n}} \left\{ \left[\frac{g}{K^{u}_{m,n} \Delta\xi} - \frac{1}{2} fruw\, l'_{m,n} \right] CC_{m+1} - \frac{\frac{1}{2} u'_{m,n} E_{m,n}}{\Delta\xi} \right\}$$

$$D_m = \frac{1}{\frac{1}{2}\Delta t} (\nu_\zeta)''_{m,n} - \left[\frac{g}{K^{u}_{m-1,n} \Delta\xi} + \frac{1}{2} fruw\, l'_{m-1,n} \right] \left[(\nu_u)''_{m-1,n} + DD_m \right] + \left[\frac{g}{K^{u}_{m,n} \Delta\xi} - \frac{1}{2} fruw\, l'_{m,n} \right] \left[(\nu_u)''_{m,n} + DD_{m+1} \right] - \frac{\frac{1}{2} u'_{m,n} E_{m,n}}{\Delta\xi} \left[\frac{(\nu_\zeta)''_{m,n}}{K^{\eta}_{m,n} E^{\xi}_{m,n}} - \frac{(\nu_\zeta)''_{m+1,n}}{K^{\eta}_{m+1,n} E^{\xi}_{m+1,n}} \right] - \frac{\frac{1}{2} u'_{m-1,n} E_{m-1,n}}{\Delta\xi} \left[\frac{(\nu_\zeta)''_{m-1,n}}{K^{\eta}_{m-1,n} E^{\xi}_{m-1,n}} - \frac{(\nu_\zeta)''_{m,n}}{K^{\eta}_{m,n} E^{\xi}_{m,n}} \right]$$

This system of matrix equations is transformed into a tridiagonal system:

$$\begin{bmatrix} B_1 & C_1 & & & & & & \\ A_2 & B_2 & C_2 & & & & & \\ & A_3 & B_3 & C_3 & & & & \\ & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & \\ & & & & A_{mf-1} & B_{mf-1} & C_{mf-1} & \\ & & & & & A_{mf} & B_{mf} \end{bmatrix} \begin{bmatrix} (\nu_\zeta)'_{1,n} \\ (\nu_\zeta)'_{2,n} \\ (\nu_\zeta)'_{3,n} \\ \cdot \\ \cdot \\ (\nu_\zeta)'_{mf,n} \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ \cdot \\ \cdot \\ D_{mf-1} \\ D_{mf} \end{bmatrix}$$

which is written as the following equivalent system of equations:

$$\begin{bmatrix} 1 & \hat{C}_1 & & & & & \\ & 1 & \hat{C}_2 & & & & \\ & & 1 & \hat{C}_3 & & & \\ & & & \cdot & \cdot & & \\ & & & & \cdot & \cdot & \\ & & & & & 1 & \hat{C}_{mf-1} \\ & & & & & & 1 \end{bmatrix} \begin{bmatrix} (\nu_\zeta)'_{1,n} \\ (\nu_\zeta)'_{2,n} \\ (\nu_\zeta)'_{3,n} \\ \cdot \\ \cdot \\ (\nu_\zeta)'_{mf,n} \end{bmatrix} = \begin{bmatrix} \hat{D}_1 \\ \hat{D}_2 \\ \hat{D}_3 \\ \cdot \\ \cdot \\ \cdot \\ \hat{D}_{mf-1} \\ \hat{D}_{mf} \end{bmatrix}$$

$$\text{or : } (\nu_\zeta)'_{m,n} + \hat{C}_m (\nu_\zeta)'_{m+1,n} = \hat{D}_m \quad \forall m$$

These coefficients are determined recursively:

$$\hat{C}_m = \frac{C_m}{B_m - A_m \hat{C}_{m-1}}$$

$$\hat{D}_m = \frac{D_m - A_m \hat{D}_{m-1}}{B_m - A_m \hat{C}_{m-1}}$$

$$\hat{C}_1 = \frac{C_1}{B_1} \text{ and } \hat{D}_1 = \frac{D_1}{B_1}$$

Solving backwards using the same formula gives:

$$(\nu_\zeta)'_{mf,n} = \hat{D}_{mf}$$

$$(\nu_\zeta)'_{m,n} = \hat{D}_m - \hat{C}_m (\nu_\zeta)'_{m+1,n}$$

The adjoint u velocities are then calculated by substituting the adjoint water levels into the adjoint u momentum equation:

$$(\nu_u)'_{m,n} = DD_{m+1} - CC_{m+1} \left[\frac{(\nu_\zeta)'_{m+1,n}}{K^\eta_{m+1,n} E^\xi_{m+1,n}} - \frac{(\nu_\zeta)'_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} \right]$$

AD-VYD

The adjoint v momentum equation at the first stage, from t+Δt $\rightarrow$ t+½Δt, is an explicit equation:

$$\frac{1}{\frac{1}{2}\Delta t}[(\nu_v)'_{mn,} - (\nu_v)''_{m,n}] - \overline{[f_{m,n} + fruv'_{m,n}][(\nu_u)'_{m,n} + (\nu_u)''_{m,n}]}^{\xi\eta} = 0$$

The adjoint v velocities at time t+½Δt are calculated straightforwardly by substituting the adjoint v velocities at time t+Δt and the adjoint u velocities at time t+½Δt.

AD-SVU

The adjoint v momentum equation and the adjoint continuity equation at the second stage, from t+½Δt $\rightarrow$ t, are implicitly coupled equations. The adjoint v velocity at time t is expressed as a function of the unknown adjoint water levels at time t:

$$(\nu_v)_{m,n} = DD_{n+1} - CC_{n+1}\left[\frac{(\nu_\zeta)_{m,n+1}}{K^{\eta}_{m,n+1}E^{\xi}_{m,n+1}} - \frac{(\nu_\zeta)_{m,n}}{K^{\eta}_{m,n}E^{\xi}_{m,n}}\right]$$

Coefficients CC_{n+1} and DD_{n+1} are determined by:

$$CC_{n+1} = -\frac{(H^v)_{m,n}K_{m,n}}{\Delta\eta[\frac{1}{\frac{1}{2}\Delta t} + frvv_{m,n}]}$$

$$DD_{n+1} = \frac{[\frac{1}{\frac{1}{2}\Delta t} - frvv_{m,n}](\nu_v)'_{m,n}}{\frac{1}{\frac{1}{2}\Delta t} + frvv_{m,n}} - \frac{(H^v)_{m,n}K_{m,n}}{\Delta\eta[\frac{1}{\frac{1}{2}\Delta t} + frvv_{m,n}]}\left[\frac{(\nu_\zeta)'_{m,n}}{K^{\eta}_{m,n}E^{\xi}_{m,n}} - \frac{(\nu_\zeta)'_{m,n+1}}{K^{\eta}_{m,n+1}E^{\xi}_{m,n+1}}\right]$$

The adjoint v velocity at time t is eliminated from the adjoint continuity equation. This results for each row in a tridiagonal system of unknown adjoint water levels at time t:

$$A_n(\nu_\zeta)_{m,n-1} + B_n(\nu_\zeta)_{m,n} + C_n(\nu_\zeta)_{m,n+1} = D_n$$

Coefficients A_n, B_n, C_n and D_n are calculated by:

$$A_n = \frac{1}{K^{\eta}_{m,n-1} E^{\xi}_{m,n-1}} \left\{ \left[\frac{g}{E^{v}_{m,n-1} \Delta\eta} + \frac{1}{2} frvwl_{m,n-1} \right] CC_n + \frac{\frac{1}{2} v_{m,n-1} K_{m,n-1}}{\Delta\eta} \right\}$$

$$B_n = \frac{1}{K^{\eta}_{m,n} E^{\xi}_{m,n}} \left\{ \left[\frac{1}{2} frvwl_{m,n} - \frac{g}{E^{v}_{m,n} \Delta\eta} \right] CC_{n+1} - \left[\frac{g}{E^{v}_{m,n-1} \Delta\eta} + \frac{1}{2} frvwl_{m,n-1} \right] CC_n + \frac{\frac{1}{2} [v_{m,n} K_{m,n} - v_{m,n-1} K_{m,n-1}]}{\Delta\eta} \right\} + \frac{1}{\frac{1}{2} \Delta t}$$

$$C_n = \frac{1}{K^{\eta}_{m,n+1} E^{\xi}_{m,n+1}} \left\{ \left[\frac{g}{E^{v}_{m,n} \Delta\eta} - \frac{1}{2} frvwl_{m,n} \right] CC_{n+1} - \frac{\frac{1}{2} v_{m,n} K_{m,n}}{\Delta\eta} \right\}$$

$$D_n = \frac{1}{\frac{1}{2} \Delta t} (\nu_\zeta)'_{m,n} - \left[\frac{g}{E^{v}_{m,n-1} \Delta\eta} + \frac{1}{2} frvwl_{m,n-1} \right] [(\nu_v)'_{m,n-1} + DD_n] + \left[\frac{g}{E^{v}_{m,n} \Delta\eta} - \frac{1}{2} frvwl_{m,n} \right] [(\nu_v)'_{m,n} + DD_{n+1}] - \frac{\frac{1}{2} v_{m,n} K_{m,n}}{\Delta\eta} \left[\frac{(\nu_\zeta)'_{m,n}}{K^{\eta}_{m,n} E^{\xi}_{m,n}} - \frac{(\nu_\zeta)'_{m,n+1}}{K^{\eta}_{m,n+1} E^{\xi}_{m,n+1}} \right] - \frac{\frac{1}{2} v_{m,n-1} K_{m,n-1}}{\Delta\eta} \left[\frac{(\nu_\zeta)'_{m,n-1}}{K^{\eta}_{m,n-1} E^{\xi}_{m,n-1}} - \frac{(\nu_\zeta)'_{m,n}}{K^{\eta}_{m,n} E^{\xi}_{m,n}} \right]$$

If at whole time levels water level measurements have been recorded, the residuals of the observed and computed water levels are totalled to coefficient D_n.

The obtained system of matrix equations is transformed into a tridiagonal system:

$$\begin{bmatrix} B_1 & C_1 & & & & & \\ A_2 & B_2 & C_2 & & & & \\ & A_3 & B_3 & C_3 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & A_{nf-1} & B_{nf-1} & C_{nf-1} \\ & & & & & A_{nf} & B_{nf} \end{bmatrix} \begin{bmatrix} (\nu_\zeta)_{m,1} \\ (\nu_\zeta)_{m,2} \\ (\nu_\zeta)_{m,3} \\ \cdot \\ \cdot \\ \cdot \\ (\nu_\zeta)_{m,nf} \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ \cdot \\ \cdot \\ \cdot \\ D_{nf-1} \\ D_{nf} \end{bmatrix}$$

This system of equations is written as the following equivalent systems of equations:

$$\begin{bmatrix} 1 & \hat{C}_1 & & & & & \\ & 1 & \hat{C}_2 & & & & \\ & & 1 & \hat{C}_3 & & & \\ & & & \cdot & \cdot & & \\ & & & & \cdot & \cdot & \\ & & & & & 1 & \hat{C}_{nf-1} \\ & & & & & & 1 \end{bmatrix} \begin{bmatrix} (\nu_\zeta)_{m,1} \\ (\nu_\zeta)_{m,2} \\ (\nu_\zeta)_{m,3} \\ \cdot \\ \cdot \\ \cdot \\ (\nu_\zeta)_{m,nf} \end{bmatrix} = \begin{bmatrix} \hat{D}_1 \\ \hat{D}_2 \\ \hat{D}_3 \\ \cdot \\ \cdot \\ \cdot \\ \hat{D}_{nf-1} \\ \hat{D}_{nf} \end{bmatrix}$$

$$\text{or : } (\nu_\zeta)_{m,n} + \hat{C}_n (\nu_\zeta)_{m,n+1} = \hat{D}_n \quad \forall n$$

These coefficients are determined recursively:

$$\hat{C}_n = \frac{C_n}{B_n - A_n \hat{C}_{n-1}}$$

$$\hat{D}_n = \frac{D_n - A_n \hat{D}_{n-1}}{B_n - A_n \hat{C}_{n-1}}$$

$$\hat{C}_1 = \frac{C_1}{B_1} \text{ and } \hat{D}_1 = \frac{D_1}{B_1}$$

Solving backwards using the same formula gives:

$$(\nu_\zeta)_{m,nf} = \hat{D}_{nf}$$

$$(\nu_\zeta)_{m,n} = \hat{D}_n - \hat{C}_n (\nu_\zeta)_{m,n+1}$$

The adjoint v velocities are then calculated by substituting the adjoint water levels into the adjoint v momentum equation:

$$(\nu_v)_{m,n} = DD_{n+1} - CC_{n+1}\left[\frac{(\nu_\zeta)_{m,n+1}}{K^\eta_{m,n+1} E^\xi_{m,n+1}} - \frac{(\nu_\zeta)_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} \right]$$

AD-UXD

The adjoint u momentum equation at the second stage, from $t+½\Delta t \rightarrow t$, is an explicit equation:

$$\frac{1}{½\,\Delta t}[\,(\nu_u)_{m,n} - (\nu_u)'_{m,n}\,] + \overline{[f_{m,n} + frvu_{m,n}][\,(\nu_v)_{m,n} + (\nu_v)'_{m,n}\,]}^{\eta\xi} = 0$$

The adjoint v velocities at time t are calculated straightforwardly by substituting the adjoint u velocities at time $t+½\Delta t$ and the adjoint v velocities at time t.

Remarks:

- The solution method applied to solve the adjoint equations is a numerically stable method. The structure of this method is similar to the numerical method used in WAQUA. For more information on this subject see [Stelling, 1984]. Some tests regarding the numerical stability of WAQAD are described in [Mouthaan, 1992].

- If uncertain parameters of the WAQUA boundary conditions are estimated, the corresponding adjoint variables at the boundary must be calculated. The adjoint boundary conditions are solved after solving the adjoint model equations. In WAQAD the adjoint boundary conditions are solved in module AD-GRKB, see subsection 3.4.3.

- In order to reduce the computational effort, the adjoint water level in WAQAD is divided by the WAQUA transformation factors K and E in advance. The adjoint water level variable is implemented in WAQAD as:

$$(\nu_\zeta)_{m,n} := \frac{(\nu_\zeta)_{m,n}}{K^{\eta}_{m,n} E^{\xi}_{m,n}}$$

This is important when the adjoint water levels are printed or plotted as output of WAQAD.

3.3.2. Advection

This subsection describes the modifications that must be made as a result of the advective terms when solving the existing adjoint computation procedures (see subsection 3.3.1). The description is given per WAQAD module: AD-SUV, AD-VYD, AD-SVU and AD-UXD. The degenerations caused by the boundary treatment and impeded points which may inhibit the flow of water have been left out. These are discussed in appendix A.

In this subsection the advective terms are described using rectangular coordinates. For an overview of the differences between rectangular, curvilinear and spherical coordinates, see subsection 3.2.2.4.

AD-SUV

In procedure AD-SUV the adjoint conservation of mass and the adjoint u momentum equation are simultaneously solved to determine $(\nu_\zeta)'_{m,n}$ and $(\nu_u)'_{m,n}$ for all inner points in the domain of the model. In imitation of module SUV in WAQUA the adjoint u momentum equation is used to eliminate the adjoint u velocity from the adjoint conservation of mass. This leaves a tridiagonal system of equations in adjoint water levels for a row, which can be solved by the well known double sweep algorithm, [Stelling, 1984]. After this, the adjoint u momentum equations can be resolved.

Without the advective terms the adjoint u momentum equation in this stage looks like:

$$\frac{1}{\frac{1}{2}\Delta t}\left[\boxed{(\nu_u)'_{m,n}} - (\nu_u)''_{m,n} \right] + \frac{(H^u)'_{m,n}}{\Delta X}\left[\boxed{(\nu_\zeta)'_{m,n}} - \boxed{(\nu_\zeta)'_{m+1,n}} \right] \quad (3.131)$$

$$+ \frac{(H^u)'_{m,n}}{\Delta X}\left[(\nu_\zeta)''_{m,n} - (\nu_\zeta)''_{m+1,n} \right] + fruu'_{m,n}\left[\boxed{(\nu_u)'_{m,n}} + (\nu_u)''_{m,n} \right] = 0$$

Adding equation (3.100), as described in subsection (3.3.1), to the existing adjoint u momentum equation yields the same structure with other matrix coefficients:

$$\boxed{(\nu_u)'_{m,n}} = DD_{m+1,n} - CC_{m+1,n}\left[\ \boxed{(\nu_\zeta)'_{m,n}} - \boxed{(\nu_\zeta)'_{m+1,n}}\ \right] \qquad (3.132)$$

in which:

$$CC_{m+1,n} = \frac{-(H^u)'_{m,n}}{\Delta X\left[\ \frac{2}{\Delta t} + fruu'_{m,n} + \frac{(u_{m+1,n} - u_{m-1,n})}{2\Delta X}\ \right]}$$

$$DD_{m+1,n} = \frac{\left[\ \frac{2}{\Delta t} - fruu'_{m,n} - \frac{(u''_{m+1,n} - u''_{m-1,n})}{2\Delta X}\ \right](\nu_u)''_{m,n}}{\left[\ \frac{2}{\Delta t} + fruu'_{m,n} + \frac{(u_{m+1,n} - u_{m-1,n})}{2\Delta X}\ \right]}$$

$$- \frac{(H^u)'_{m,n}\left[\ (\nu_\zeta)''_{m,n} - (\nu_\zeta)''_{m+1,n}\ \right]}{\Delta X\left[\ \frac{2}{\Delta t} + fruu'_{m,n} + \frac{(u_{m+1,n} - u_{m-1,n})}{2\Delta X}\ \right]}$$

For the sake of completeness the adjoint continuity equation (advection included) associated with $\Delta\zeta'_{m,n}$ will also be given:

$$\frac{2}{\Delta t}\left[\ \boxed{(\nu_\zeta)'_{m,n}} - (\nu_\zeta)''_{m,n}\ \right]$$

$$+ \frac{g}{\Delta X}\left[\ -(\nu_u)''_{m,n} - \boxed{(\nu_u)'_{m,n}} + (\nu_u)''_{m-1,n} + \boxed{(\nu_u)'_{m-1,n}}\ \right]$$

$$+ \frac{\frac{1}{2}u'_{m,n}}{\Delta X}\left[\ \boxed{(\nu_\zeta)'_{m,n}} + (\nu_\zeta)''_{m,n} - \boxed{(\nu_\zeta)'_{m+1,n}} - (\nu_\zeta)''_{m+1,n}\ \right] \qquad (3.133)$$

$$+ \frac{\frac{1}{2}u'_{m-1,n}}{\Delta X}\left[\ -\boxed{(\nu_\zeta)'_{m,n}} - (\nu_\zeta)''_{m,n} + \boxed{(\nu_\zeta)'_{m-1,n}} + (\nu_\zeta)''_{m-1,n}\ \right]$$

$$+ \overline{fruwl'_{m-1,n}}\left[\ \overline{\boxed{(\nu_u)'_{m-1,n}} + (\nu_u)''_{m-1,n}}\ \right]^{\xi} = 0$$

In this equation three adjoint water levels and two adjoint u velocities at the new time level occur. They form a pentadiagonal matrix equation together with the adjoint u momentum equation if the corresponding equations for all grid points in a row of the domain are written down.

$$\begin{array}{ccccccccccc}
(\nu_\zeta) & (\nu_u)_{m-2} & (\nu_\zeta) & & & & & & & & \\
(\nu_\zeta) & (\nu_u) & (\nu_\zeta)_{m-1} & (\nu_u) & (\nu_\zeta) & & & & & & \\
 & & (\nu_\zeta) & (\nu_u)_{m-1} & (\nu_\zeta) & & & & & & \\
 & & (\nu_\zeta) & (\nu_u) & (\nu_\zeta)_m & (\nu_u) & (\nu_\zeta) & & & & \\
 & & & & (\nu_\zeta) & (\nu_u)_m & (\nu_\zeta) & & & & \\
 & & & & (\nu_\zeta) & (\nu_u) & (\nu_\zeta)_{m+1} & (\nu_u) & (\nu_\zeta) & & \\
 & & & & & & (\nu_\zeta) & (\nu_u)_{m+1} & (\nu_\zeta) & &
\end{array} \qquad (3.134)$$

The adjoint u contributions in the adjoint continuity equation are eliminated by means of the adjoint u momentum equation with a substitution. The result is a tridiagonal matrix equation for each row consisting of adjoint ζ contributions:

$$\begin{array}{ccccc}
(\nu_\zeta) & (\nu_\zeta)_{m-1} & (\nu_\zeta) & & \\
 & (\nu_\zeta) & (\nu_\zeta)_m & (\nu_\zeta) & \\
 & & (\nu_\zeta) & (\nu_\zeta)_{m+1} & (\nu_\zeta) \\
 & & & (\nu_\zeta) & (\nu_\zeta)_{m+2}\ (\nu_\zeta)
\end{array} \qquad (3.135)$$

This matrix equation is solved with Gaussian elimination (double sweep method), [Stelling, 1984]. The adjoint u momentum equation can then subsequently be solved by simple substitution.

AD-VYD

In procedure AD-VYD the adjoint v momentum equation is solved to determine $(\nu_v)'_{m,n}$ for all inner points of the domain of the model. So far the adjoint advective terms have been omitted. The existing adjoint v momentum equation at this first stage of the adjoint computation process reads:

$$\frac{1}{\frac{1}{2}\Delta t}\left[(\nu_v)'_{m,n} - (\nu_v)''_{M,N} \right] - \left[f_{m,n} + fruv'_{m,n} \right] \overline{\left[(\nu_u)'_{m,n} + (\nu_u)''_{m,n} \right]}^{\xi\eta} = 0 \qquad (3.136)$$

Without the advective terms a diagonal matrix equation over a grid line in y direction is obtained:

$$B_{m,n}\,(\nu_v)'_{m,n} = D_{m,n} \tag{3.137}$$

in which:

$$B_{m,n} = \frac{2}{\Delta t}$$

$$D_{m,n} = \frac{2}{\Delta t}(\nu_v)''_{m,n} + \overline{[f_{m,n} - fru'_{m,n}]\,[(\nu_u)'_{m,n} + (\nu_u)''_{m,n}]}^{\xi\eta}$$

Adding (3.101) ··· (3.104) (omitting (3.105)) to this existing adjoint v momentum equation yields a tridiagonal matrix equation for a column in the domain of the model:

$$\begin{array}{ccccc} (\nu_v) & (\nu_v)_{n-1} & (\nu_v) & & \\ & (\nu_v) & (\nu_v)_n & (\nu_v) & \\ & & (\nu_v) & (\nu_v)_{n+1} & (\nu_v) \\ & & & (\nu_v) & (\nu_v)_{n+2} \quad (\nu_v) \end{array} \tag{3.138}$$

This banded system could be solved over the grid lines in y direction by standard procedures. The corresponding coefficients of this matrix equation are:

$$A_{m,n}\ \boxed{(\nu_v)'_{m,n-1}} + B_{m,n}\ \boxed{(\nu_v)'_{m,n}} + C_{m,n}\ \boxed{(\nu_v)'_{m,n+1}} = D_{m,n} \quad (3.139)$$

in which:

$$A_{m,n} = \frac{v_{m,n-1}}{2\Delta Y} \quad (3.140)$$

$$B_{m,n} = B_{m,n} \quad (3.141)$$

$$C_{m,n} = \frac{-v_{m,n+1}}{2\Delta Y} \quad (3.142)$$

$$D_{m,n} = D_{m,n} \quad (3.143)$$

$$-\frac{\left(v''_{m,n-1}(\nu_v)''_{m,n-1} - v''_{m,n+1}(\nu_v)''_{m,n+1}\right)}{2\Delta Y} \quad (3.144)$$

$$\begin{aligned} &-(\nu_v)''_{m-2,n}\left(\frac{\overline{\overline{u''}}_{m-2,n}}{12\Delta X}\right) - (\nu_v)''_{m-1,n}\left(\frac{4\overline{\overline{u''}}_{m-1,n}}{12\Delta X}\right) \\ &+(\nu_v)''_{m+1,n}\left(\frac{4\overline{\overline{u''}}_{m+1,n}}{12\Delta X}\right) + (\nu_v)''_{m+2,n}\left(\frac{\overline{\overline{u''}}_{m+2,n}}{12\Delta X}\right) \end{aligned} \quad (3.145)$$

$$\begin{aligned} &-(\nu_u)''_{m,n}\tfrac{1}{4}S^u_y(u''_{m,n}) - (\nu_u)''_{m-1,n}\tfrac{1}{4}S^u_y(u''_{m-1,n}) \\ &-(\nu_u)''_{m-1,n+1}\tfrac{1}{4}S^u_y(u''_{m-1,n+1}) - (\nu_u)''_{m,n+1}\tfrac{1}{4}S^u_y(u''_{m,n+1}) \end{aligned} \quad (3.146)$$

$$\begin{aligned} &-(\nu_u)'_{m,n}\tfrac{1}{4}S^c_y(u_{m,n}) - (\nu_u)'_{m-1,n}\tfrac{1}{4}S^c_y(u_{m-1,n}) \\ &-(\nu_u)'_{m-1,n+1}\tfrac{1}{4}S^c_y(u_{m-1,n+1}) - (\nu_u)'_{m,n+1}\tfrac{1}{4}S^c_y(u_{m,n+1}) \end{aligned} \quad (3.147)$$

Remark: Note that the coefficients A, B, C and D that are calculated in module ADSUV are not the same as those calculated in module ADVYD.

Adding equation (3.105) to equation (3.139) yields:

$$B_{m,n} = B_{m,n} \tag{3.148}$$

$$+ \left(\frac{-3\overline{\overline{u}}_{m,n}}{2\Delta X} \right) \quad \text{if } \overline{\overline{u}}_{m,n} \le 0,$$

$$+ \left(\frac{3\overline{\overline{u}}_{m,n}}{2\Delta X} \right) \quad \text{if } \overline{\overline{u}}_{m,n} > 0$$

Adding equation (3.105) to equations (3.143) to (3.147) yields:

$$D_{m,n} = D_{m,n} \tag{3.149}$$

$$- \boxed{(\nu_v)'_{m-2,n}} \left(\frac{-\overline{\overline{u}}_{m-2,n}}{2\Delta X} \right) \quad \text{if } \overline{\overline{u}}_{m-2,n} \le 0,$$

$$- \boxed{(\nu_v)'_{m-1,n}} \left(\frac{4\overline{\overline{u}}_{m-1,n}}{2\Delta X} \right) \quad \text{if } \overline{\overline{u}}_{m-1,n} \le 0,$$

$$- \boxed{(\nu_v)'_{m+1,n}} \left(\frac{-4\overline{\overline{u}}_{m+1,n}}{2\Delta X} \right) \quad \text{if } \overline{\overline{u}}_{m+1,n} > 0,$$

$$- \boxed{(\nu_v)'_{m+2,n}} \left(\frac{\overline{\overline{u}}_{m+2,n}}{2\Delta X} \right) \quad \text{if } \overline{\overline{u}}^{k}_{m+2,n} > 0$$

The system is solved iteratively using a Jacobi method. The computed values from the previous loop are used to compute the marked adjoint variables in equation (3.149) .

AD-SVU

In procedure AD-SVU the adjoint conservation of mass and the adjoint v momentum equation are simultaneously solved to determine (ν_ζ) and (ν_v). Since this computation procedure is analogous to the procedure AD-SUV, only the important formulas will be given below.

Without the advective terms the existing adjoint v momentum equation at this stage looks like:

$$\frac{1}{\frac{1}{2}\Delta t}\left[\boxed{(\nu_v)_{m,n}} - (\nu_v)'_{m,n}\right] + \frac{(H^v)_{m,n}}{\Delta Y}\left[\boxed{(\nu_\zeta)'_{m,n}} - \boxed{(\nu_\zeta)'_{m,n+1}}\right] \quad (3.150)$$

$$+ \frac{(H^v)_{m,n}}{\Delta Y}\left[(\nu_\zeta)_{m,n} - (\nu_\zeta)_{m,n+1}\right] + frvv_{m,n}\left[\boxed{(\nu_v)_{m,n}} + (\nu_v)'_{m,n}\right] = 0$$

Adding (3.106) to this existing adjoint v momentum equation results in the same matrix structure:

$$\boxed{(\nu_v)_{m,n}} = DD_{m,n+1} - CC_{m,n+1}\left[\boxed{(\nu_\zeta)_{m,n+1}} - \boxed{(\nu_\zeta)_{m,n}}\right] \quad (3.151)$$

in which:

$$CC_{m,n+1} = \frac{-(H^v)_{m,n}}{\Delta Y\left[\frac{2}{\Delta t} + frvv_{m,n} + \frac{\left(\bar{v}'_{m,n+1} - \bar{v}'_{m,n-1}\right)}{2\Delta Y}\right]}$$

$$DD_{m,n+1} = \frac{\left[\frac{2}{\Delta t} - frvv_{m,n} - \frac{\left(v'_{m,n+1} - v'_{m,n-1}\right)}{2\Delta Y}\right](\nu_v)'_{m,n}}{\left[\frac{2}{\Delta t} + frvv_{m,n} + \frac{\left(\bar{v}'_{m,n+1} - \bar{v}'_{m,n-1}\right)}{2\Delta Y}\right]}$$

$$- \frac{(H^v)_{m,n}\left[(\nu_\zeta)'_{m,n} - (\nu_\zeta)'_{m,n+1}\right]}{\Delta Y\left[\frac{2}{\Delta t} + frvv_{m,n} + \frac{\left(\bar{v}'_{m,n+1} - \bar{v}'_{m,n-1}\right)}{2\Delta Y}\right]}$$

For the sake of completeness, here is the adjoint continuity equation associated with $\Delta\zeta_{m,n}$:

$$\frac{2}{\Delta t}[\ (\nu_\zeta)_{m,n} - (\nu_\zeta)'_{m,n}\ ]$$

$$+\frac{g}{\Delta Y}[\ -(\nu_v)'_{m,n} - (\nu_v)_{m,n} + (\nu_v)'_{m,n-1} + (\nu_v)_{m,n-1}\ ]$$

$$+\frac{\frac{1}{2}V_{m,n}}{\Delta Y}[\ (\nu_\zeta)_{m,n} + (\nu_\zeta)'_{m,n} - (\nu_\zeta)_{m,n+1} - (\nu_\zeta)'_{m,n+1}\ ] \quad (3.152)$$

$$+\frac{\frac{1}{2}V_{m,n-1}}{\Delta Y}[\ -(\nu_\zeta)_{m,n} - (\nu_\zeta)'_{m,n} + (\nu_\zeta)_{m,n-1} + (\nu_\zeta)'_{m,n-1}\ ]$$

$$+\overline{frvwl}_{m,n}[\ \overline{(\nu_v)_{m,n}} + \overline{(\nu_v)'_{m,n}}\ ]^{\eta} = 0$$

In (3.152) three adjoint water levels and two adjoint v velocities at the new time level occur. Together with this adjoint v momentum equation they form a pentadiagonal matrix equation, if for all grid points in a column of the domain the corresponding equations are written down:

$$\begin{array}{ccccccccc}
(\nu_\zeta) & (\nu_v)_{n-2} & (\nu_\zeta) & & & & & & \\
(\nu_\zeta) & (\nu_v) & (\nu_\zeta)_{n-1} & (\nu_v) & (\nu_\zeta) & & & & \\
 & & (\nu_\zeta) & (\nu_v)_{n-1} & (\nu_\zeta) & & & & \\
 & & (\nu_\zeta) & (\nu_v) & (\nu_\zeta)_n & (\nu_v) & (\nu_\zeta) & & \\
 & & & & (\nu_\zeta) & (\nu_v)_n & (\nu_\zeta) & & \\
 & & & & (\nu_\zeta) & (\nu_v) & (\nu_\zeta)_{n+1} & (\nu_v) & (\nu_\zeta) \\
 & & & & & & (\nu_\zeta) & (\nu_v)_{n+1} & (\nu_\zeta)
\end{array} \quad (3.153)$$

The adjoint v contributions in the adjoint continuity equation are eliminated by means of the adjoint v momentum equation with a substitution. The result is a tridiagonal matrix equation for each column, consisting solely of adjoint ζ contributions:

$$\begin{array}{ccccccc}
(\nu_\zeta) & (\nu_\zeta)_{n-1} & (\nu_\zeta) & & & & \\
 & (\nu_\zeta) & (\nu_\zeta)_n & (\nu_\zeta) & & & \\
 & & (\nu_\zeta) & (\nu_\zeta)_{n+1} & (\nu_\zeta) & & \\
 & & & (\nu_\zeta) & (\nu_\zeta)_{n+2} & (\nu_\zeta)
\end{array} \quad (3.154)$$

This matrix equation is solved with Gaussian elimination (double sweep method), [Stelling, 1984]. The adjoint v

momentum equation can then be solved by simple substitution.

AD-UXD

In procedure AD-UXD the adjoint u momentum equation is solved to determine $(\nu_u)_{m,n}$. The existing adjoint u momentum equation at this second stage of the adjoint computation process reads:

$$\frac{1}{\frac{1}{2}\Delta t}\left[\boxed{(\nu_u)_{m,n}} - (\nu_u)'_{m,n}\right] + \overline{\left[f_{m,n} + frvu_{m,n}\right]\left[(\nu_v)_{m,n} + (\nu_v)'_{m,n}\right]}^{\eta\xi} = 0 \tag{3.155}$$

Without the advective terms, diagonal matrix equations over a grid line in x direction are obtained:

$$B_{m,n}\boxed{(\nu_u)_{m,n}} = D_{m,n} \tag{3.156}$$

in which:

$$B_{m,n} = \frac{2}{\Delta t}$$

$$D_{m,n} = \frac{2}{\Delta t}(\nu_u)'_{m,n} - \overline{\left[f_{m,n} - frvu_{m,n}\right]\left[(\nu_v)_{m,n} + (\nu_v)'_{m,n}\right]}^{\eta\xi}$$

Adding (3.107) ··· (3.110) (omitting (3.111)) to this existing adjoint u momentum equation yields a tridiagonal matrix equation for a row in the domain of the model.

$$\begin{array}{cccccc} (\nu_u) & (\nu_u)_{m-1} & (\nu_u) & & & \\ & (\nu_u) & (\nu_u)_m & (\nu_u) & & \\ & & (\nu_u) & (\nu_u)_{m+1} & (\nu_u) & \\ & & & (\nu_u) & (\nu_u)_{m+2} & (\nu_u) \end{array} \tag{3.157}$$

This banded system could be solved over the gridlines in x direction by standard procedures. The corresponding coefficients of this matrix equation are:

$$A_{m,n}\ \boxed{(\nu_u)_{m-1,n}} + B_{m,n}\ \boxed{(\nu_u)_{m,n}} + C_{m,n}\ \boxed{(\nu_u)_{m+1,n}} = D_{m,n} \quad (3.158)$$

in which:

$$A_{m,n} = \frac{\bar{u}'_{m-1,n}}{2\Delta X} \quad (3.159)$$

$$B_{m,n} = B_{m,n} \quad (3.160)$$

$$C_{m,n} = \frac{-\bar{u}'_{m+1,n}}{2\Delta X} \quad (3.161)$$

$$D_{m,n} = D_{m,n} \quad (3.162)$$

$$-\frac{\left(u'_{m-1,n}(\nu_u)'_{m-1,n} - u'_{m+1,n}(\nu_u)'_{m+1,n} \right)}{2\Delta X} \quad (3.163)$$

$$\begin{aligned} &-(\nu_u)'_{m,n-2}\left(\frac{\bar{\bar{v}}'_{m,n-2}}{12\Delta Y}\right) - (\nu_u)'_{m,n-1}\left(\frac{4\bar{\bar{v}}'_{m,n-1}}{12\Delta Y}\right) \\ &+(\nu_u)'_{m,n+1}\left(\frac{4\bar{\bar{v}}'_{m,n+1}}{12\Delta Y}\right) + (\nu_u)'_{m,n+2}\left(\frac{\bar{\bar{v}}'_{m,n+2}}{12\Delta Y}\right) \end{aligned} \quad (3.164)$$

$$\begin{aligned} &-(\nu_v)'_{m,n}\tfrac{1}{4}S^u_x(v'_{m,n}) - (\nu_v)'_{m+1,n}\tfrac{1}{4}S^u_x(v'_{m+1,n}) \\ &-(\nu_v)'_{m+1,n-1}\tfrac{1}{4}S^u_x(v_{m+1,n-1}) - (\nu_v)'_{m,n-1}\tfrac{1}{4}S^u_x(v'_{m,n-1}) \end{aligned} \quad (3.165)$$

$$\begin{aligned} &-(\nu_v)_{m,n}\tfrac{1}{4}S^c_x(\bar{v}'_{m,n}) - (\nu_v)_{m+1,n}\tfrac{1}{4}S^c_x(\bar{v}'_{m+1,n}) \\ &-(\nu_v)_{m+1,n-1}\tfrac{1}{4}S^c_x(\bar{v}'_{m+1,n-1}) - (\nu_v)_{m,n-1}\tfrac{1}{4}S^c_x(\bar{v}'_{m,n-1}) \end{aligned} \quad (3.166)$$

Remark: Note that the coefficients A, B, C and D that are calculated in module ADSVU are not the same as those calculated in module ADUXD.

Adding equation (3.111) to equation (3.158) yields:

$$B_{m,n} = B_{m,n} \tag{3.167}$$

$$+ \left(\frac{3\overline{\overline{v}}_{m,n}}{2\Delta Y} \right) \qquad \text{if } \overline{\overline{v}}_{m,n} > 0 ,$$

$$+ \left(\frac{-3\overline{\overline{v}}_{m,n}}{2\Delta Y} \right) \qquad \text{if } \overline{\overline{v}}_{m,n} \le 0$$

Adding equation (3.111) to equations (3.163) to (3.166) yields:

$$D_{m,n} = D_{m,n} \tag{3.168}$$

$$- \boxed{(\nu_u)_{m,n+2}} \left(\frac{\overline{\overline{v}}_{m,n+2}}{2\Delta Y} \right) \quad \text{if } \overline{\overline{v}}_{m,n+2} > 0$$

$$- \boxed{(\nu_u)_{m,n+1}} \left(\frac{-4\overline{\overline{v}}_{m,n+1}}{2\Delta Y} \right) \quad \text{if } \overline{\overline{v}}_{m,n+1} > 0$$

$$- \boxed{(\nu_u)_{m,n-1}} \left(\frac{4\overline{\overline{v}}_{m,n-1}}{2\Delta Y} \right) \quad \text{if } \overline{\overline{v}}_{m,n-1} \le 0$$

$$- \boxed{(\nu_u)_{m,n-2}} \left(\frac{-\overline{\overline{v}}_{m,n-2}}{2\Delta Y} \right) \quad \text{if } \overline{\overline{v}}_{m,n-2} \le 0$$

The system is solved iteratively using a Jacobi method. The computed values from the previous loop are used to compute the marked adjoint variables in equation (3.168).

3.3.3. Dryfall

In this subsection an overview of the drying procedures in the WAQAD modules AD-SUV, AD-VYD, AD-SVU and AD-UXD is given.

AD-SUV

If dryfall occurs in WAQUA in the first stage (from $t \rightarrow t+½\Delta t$) at a u velocity point, then the corresponding u velocity point in WAQAD in the first stage (from $t+\Delta t \rightarrow t+½\Delta t$) must fall dry. This means that at this stage the system of equations must be solved, considering this point as a closed WAQAD boundary condition. Instead of solving the adjoint u momentum equation, the adjoint u velocity is set to equal zero.

AD-VYD

If dryfall occurs in WAQUA in the first stage (from $t \rightarrow t+½\Delta t$) at a v velocity point, then the corresponding v velocity point in WAQAD in the first stage (from $t+\Delta t \rightarrow t+½\Delta t$) must fall dry. In short: the adjoint v velocity is set to equal zero.

AD-SVU

If dryfall occurs in WAQUA in the second stage (from t-½Δt $\rightarrow$ t) at a v velocity point, then the corresponding v velocity point in WAQAD in the second stage (from t+½Δt $\rightarrow$ t) must fall dry. In short: the adjoint v velocity is set to equal zero.

AD-UXD

If dryfall occurs in WAQUA in the second stage (from t-½Δt $\rightarrow$ t) at a u velocity point, then the corresponding u velocity point in WAQAD in the second stage (from t+½Δt $\rightarrow$ t) must fall dry. In short: the adjoint u velocity is set to equal zero.

3.4. The gradient

When the adjoint model equations are solved, the gradient can be calculated with this solution. In the following subsections the expression of the gradient is derived for three cases:

- the parameter to be estimated is a correction factor for the bottom friction coefficient, subsection 3.4.1.
- the parameter to be estimated is a correction factor for the depth, subsection 3.4.2.
- the parameters to be estimated are correction factors for the amplitude and phase of the boundary condition, subsection 3.4.3.

3.4.1. Bottom friction

In this subsection the expression of the gradient for bottom friction is derived. The parameter to be estimated is a correction factor for the Chezy coefficient at u velocity point (m,n) and v velocity point (m,n). For bottom friction in the case of Manning and White Colebrook, see section 5.6.

An overview of the contributions of the WAQUA u and v momentum equations is given first. Then the expression of the gradient is deduced.

- Contribution of the WAQUA v momentum equation in the first stage (from $t \rightarrow t+½\Delta t$) at point (m,n):

$$(\nu_v)'_{m,n}\left[\frac{-2g}{(C^v_{m,n})^3}\frac{v_{m,n}\sqrt{(\overline{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}}{D^v_{m,n}+\overline{\zeta}^{\eta}_{m,n}}\right]$$

- Contribution of the WAQUA u momentum equation in the first stage (from $t \rightarrow t+½\Delta t$) at point (m,n):

$$(\nu_u)'_{m,n}\left[\frac{-2g}{(C^u_{m,n})^3}\frac{u'_{m,n}\sqrt{(u'_{m,n})^2+(\overline{v}'^{\eta\xi}_{m,n})^2}}{D^u_{m,n}+\overline{\zeta}'^{\xi}_{m,n}}\right]$$

- Contribution of the WAQUA u momentum equation in the second stage (from $t+½\Delta t$ $t+\Delta t$) at point (m,n):

$$(\nu_u)''_{m,n}\left[\frac{-2g}{(C^u_{m,n})^3}\frac{u'_{m,n}\sqrt{(u'_{m,n})^2+(\overline{v}'^{\eta\xi}_{m,n})^2}}{D^u_{m,n}+\overline{\zeta}'^{\xi}_{m,n}}\right]$$

- Contribution of the WAQUA v momentum equation in the second stage (from t+½Δt t+Δt) at point (m,n):

$$(\nu_v)''_{m,n}\left[\frac{-2g}{(C^v_{m,n})^3}\frac{v''_{m,n}\sqrt{(\overline{u''}^{\xi\eta}_{m,n})^2+(v''_{m,n})^2}}{D^v_{m,n}+\overline{\zeta''}^{\eta}_{m,n}}\right]$$

The expression of the gradient for bottom friction in the first stage becomes:

$$-2^*\sum_{m,n,k}\left\{(\nu_v)'_{m,n}\left[\frac{g}{(C^v_{m,n})^3}\frac{v_{m,n}\sqrt{(\overline{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}}{D^v_{m,n}+\overline{\zeta}^{\eta}_{m,n}}\right]+(\nu_u)'_{m,n}\left[\frac{g}{(C^u_{m,n})^3}\frac{u_{m',n}\sqrt{(u'_{m,n})^2+(\overline{v'}^{\eta\xi}_{m,n})^2}}{D^u_{m,n}+\overline{\zeta'}^{\xi}_{m,n}}\right]\right\}$$

And the expression of the gradient for bottom friction in the second stage becomes:

$$-2^*\sum_{m,n,k}\left\{(\nu_u)_{m,n}\left[\frac{g}{(C^u_{m,n})^3}\frac{u'_{m,n}\sqrt{(u'_{m,n})^2+(\overline{v'}^{\eta\xi}_{m,n})^2}}{D^u_{m,n}+\overline{\zeta'}^{\xi}_{m,n}}\right]+(\nu_v)_{m,n}\left[\frac{g}{(C^v_{m,n})^3}\frac{v_{m,n}\sqrt{(\overline{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}}{D^v_{m,n}+\overline{\zeta}^{\eta}_{m,n}}\right]\right\}$$

The gradient for bottom friction is calculated in WAQAD module AD-GRCZ.

3.4.2. Depth

In this subsection the expression of the gradient for depth is derived. The parameter to be estimated is a correction factor for the depth in point (m,n).

An overview of the contributions of the WAQUA momentum equations and the WAQUA continuity equation is given first. Then the expression of the gradient is deduced.

- Contribution of the WAQUA v momentum equation in the first stage (from $t \rightarrow t+½\Delta t$) at point(m,n):

$$(\nu_v)'_{m,n}\left[\frac{-g}{2(C^v_{m,n})^2}\frac{v_{m,n}\sqrt{(\overline{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}}{(D^v_{m,n}+\overline{\zeta}^{\eta}_{m,n})^2}\right]$$

- Contribution of the WAQUA v momentum equation in the first stage (from $t \rightarrow t+½\Delta t$) at point (m+1,n):

$$(\nu_v)'_{m+1,n}\left[\frac{-g}{2(C^v_{m+1,n})^2}\frac{v_{m+1,n}\sqrt{(\overline{u}^{\xi\eta}_{m+1,n})^2+(v_{m+1,n})^2}}{(D^v_{m+1,n}+\overline{\zeta}^{\eta}_{m+1,n})^2}\right]$$

- Contribution of the WAQUA u momentum equation in the first stage (from $t \rightarrow t+½\Delta t$) at point (m,n):

$$(\nu_u)'_{m,n}\left[\frac{-g}{2(C^u_{m,n})^2}\frac{u'_{m,n}\sqrt{(u'_{m,n})^2+(\overline{v'}^{\eta\xi}_{m,n})^2}}{(D^u_{m,n}+\overline{\zeta'}^{\xi}_{m,n})^2}\right]$$

- Contribution of the WAQUA u momentum equation in the first stage (from $t \rightarrow t+½\Delta t$) at point (m,n+1):

$$(\nu_u)'_{m,n+1}\left[\frac{-g}{2(C^u_{m,n+1})^2}\frac{u'_{m,n+1}\sqrt{(u'_{m,n+1})^2+(\overline{v'}^{\eta\xi}_{m,n+1})^2}}{(D^u_{m,n+1}+\overline{\zeta'}^{\xi}_{m,n+1})^2}\right]$$

- Contribution of the WAQUA continuity equation in the first stage (from $t \rightarrow t+½\Delta t$) at point (m,n):

$$\frac{(\nu_\zeta)'_{m,n}}{K^{\eta}_{m,n}E^{\xi}_{m,n}}\left[\frac{\frac{1}{2}u'_{m,n}E_{m,n}}{\Delta\xi}+\frac{\frac{1}{2}v_{m,n}K_{m,n}}{\Delta\eta}\right]$$

- Contribution of the WAQUA continuity equation in the first stage (from $t \rightarrow t+½\Delta t$) at point (m+1,n):

$$\frac{(\nu_\zeta)'_{m+1,n}}{K^{\eta}_{m+1,n}E^{\xi}_{m+1,n}}\left[\frac{-\frac{1}{2}u'_{m,n}E_{m,n}}{\Delta\xi}+\frac{\frac{1}{2}v_{m+1,n}K_{m+1,n}}{\Delta\eta}\right]$$

- Contribution of the WAQUA continuity equation in the first stage (from $t \rightarrow t+½\Delta t$) at point (m+1,n+1):

$$\frac{(\nu_\zeta)'_{m+1,n+1}}{K^{\eta}_{m+1,n+1}E^{\xi}_{m+1,n+1}}\left[\frac{-\frac{1}{2}u'_{m,n+1}E_{m,n+1}}{\Delta\xi}+\frac{-\frac{1}{2}v_{m+1,n}K_{m+1,n}}{\Delta\eta}\right]$$

- Contribution of the WAQUA continuity equation in the first stage (from $t \rightarrow t+½\Delta t$) at point (m,n+1):

$$\frac{(\nu_\zeta)'_{m,n+1}}{K^\eta_{m,n+1}E^\xi_{m,n+1}}\left[\frac{\frac{1}{2}u'_{m,n+1}E_{m,n+1}}{\Delta\xi}+\frac{-\frac{1}{2}v_{m,n}K_{m,n}}{\Delta\eta}\right]$$

- Contribution of the WAQUA u momentum equation in the second stage (from $t+½\Delta t \rightarrow t+\Delta t$) at point (m,n):

$$(\nu_u)''_{m,n}\left[\frac{-g}{2(C^u_{m,n})^2}\frac{u'_{m,n}\sqrt{(u'_{m,n})^2+(\overline{v'}^{\eta\xi}_{m,n})^2}}{(D^u_{m,n}+\overline{\zeta'}^{\xi}_{m,n})^2}\right]$$

- Contribution of the WAQUA u momentum equation in the second stage (from $t+½\Delta t \rightarrow t+\Delta t$) at point (m,n+1):

$$(\nu_u)''_{m,n+1}\left[\frac{-g}{2(C^u_{m,n+1})^2}\frac{u'_{m+1,n}\sqrt{(u'_{m,n+1})^2+(\overline{v'}^{\eta\xi}_{m,n+1})^2}}{(D^u_{m,n+1}+\overline{\zeta'}^{\xi}_{m,n+1})^2}\right]$$

- Contribution of the WAQUA v momentum equation in the second stage (from $t+½\Delta t \rightarrow t+\Delta t$) at point (m,n):

$$(\nu_v)''_{m,n}\left[\frac{-g}{2(C^v_{m,n})^2}\frac{v''_{m,n}\sqrt{(\overline{u''}^{\xi\eta}_{m,n})^2+(v''_{m,n})^2}}{(D^v_{m,n}+\overline{\zeta''}^{\eta}_{m,n})^2}\right]$$

- Contribution of the WAQUA v momentum equation in the second stage (from $t+½\Delta t \rightarrow t+\Delta t$) at point (m+1,n):

$$(\nu_v)''_{m+1,n}\left[\frac{-g}{2(C^v_{m+1,n})^2}\frac{v''_{m+1,n}\sqrt{(\overline{u''}^{\xi\eta}_{m+1,n})^2+(v''_{m+1,n})^2}}{(D^v_{m+1,n}+\overline{\zeta''}^{\eta}_{m+1,n})^2}\right]$$

- Contribution of the WAQUA continuity equation in the second stage (from $t+½\Delta t \rightarrow t+\Delta t$) at point (m,n):

$$\frac{(\nu_\zeta)''_{m,n}}{K^\eta_{m,n}E^\xi_{m,n}}\left[\frac{\frac{1}{2}u'_{m,n}E_{m,n}}{\Delta\xi}+\frac{\frac{1}{2}v''_{m,n}K_{m,n}}{\Delta\eta}\right]$$

- Contribution of the WAQUA continuity equation in the second stage (from $t+½\Delta t \rightarrow t+\Delta t$) at point (m+1,n):

$$\frac{(\nu_\zeta)''_{m+1,n}}{K^\eta_{m+1,n}E^\xi_{m+1,n}}\left[\frac{-\frac{1}{2}u'_{m,n}E_{m,n}}{\Delta\xi}+\frac{\frac{1}{2}v''_{m+1,n}K_{m+1,n}}{\Delta\eta}\right]$$

- Contribution of the WAQUA continuity equation in the second stage (from $t+\frac{1}{2}\Delta t \rightarrow t+\Delta t$) at point (m+1,n+1):

$$\frac{(\nu_\zeta)''_{m+1,n+1}}{K^\eta_{m+1,n+1}E^\xi_{m+1,n+1}}\left[\frac{-\frac{1}{2}u'_{m,n+1}E_{m,n+1}}{\Delta\xi}+\frac{-\frac{1}{2}v''_{m+1,n}K_{m+1,n}}{\Delta\eta}\right]$$

- Contribution of the WAQUA continuity equation in the second stage (from $t+\frac{1}{2}\Delta t \rightarrow t+\Delta t$) at point (m,n+1):

$$\frac{(\nu_\zeta)''_{m,n+1}}{K^\eta_{m,n+1}E^\xi_{m,n+1}}\left[\frac{\frac{1}{2}u'_{m,n+1}E_{m,n+1}}{\Delta\xi}+\frac{-\frac{1}{2}v''_{m,n}K_{m,n}}{\Delta\eta}\right]$$

The expression of the gradient for depth in the first stage becomes:

$$\frac{1}{2}*\sum_{m,n,k}\Big\{(\nu_u)'_{m,n}\,fruwl'_{m,n}+(\nu_u)'_{m,n+1}\,fruwl_{m,n+1}+$$

$$(\nu_u)_{m,n}\,fruwl^{-'}_{m,n}+(\nu_u)_{m,n+1}\,fruwl^{-'}_{m,n+1}+$$

$$\frac{(\nu_\zeta)'_{m,n}}{K^\eta_{m,n}E^\xi_{m,n}}\left(\frac{u'_{m,n}E_{m,n}}{\Delta\xi}\right)+\frac{(\nu_\zeta)'_{m+1,n}}{K^\eta_{m+1,n}E^\xi_{m+1,n}}\left(\frac{-u'_{m,n}E_{m,n}}{\Delta\xi}\right)+$$

$$\frac{(\nu_\zeta)'_{m+1,n+1}}{K^\eta_{m+1,n+1}E^\xi_{m+1,n+1}}\left(\frac{-u'_{m,n+1}E_{m,n+1}}{\Delta\xi}\right)+\frac{(\nu_\zeta)'_{m,n+1}}{K^\eta_{m,n+1}E^\xi_{m,n+1}}\left(\frac{u'_{m,n+1}E_{m,n+1}}{\Delta\xi}\right)+$$

$$\frac{(\nu_\zeta)'_{m,n}}{K^\eta_{m,n}E^\xi_{m,n}}\left(\frac{v_{m,n}K_{m,n}}{\Delta\eta}\right)+\frac{(\nu_\zeta)'_{m+1,n}}{K^\eta_{m+1,n}E^\xi_{m+1,n}}\left(\frac{v_{m+1,n}K_{m+1,n}}{\Delta\eta}\right)+$$

$$\frac{(\nu_\zeta)'_{m+1,n+1}}{K^\eta_{m+1,n+1}E^\xi_{m+1,n+1}}\left(\frac{-v_{m+1,n}K_{m+1,n}}{\Delta\eta}\right)+\frac{(\nu_\zeta)'_{m,n+1}}{K^\eta_{m,n+1}E^\xi_{m,n+1}}\left(\frac{-v_{m,n}K_{m,n}}{\Delta\eta}\right)\Big\}$$

And the expression of the gradient for depth in the second stage becomes:

$$\frac{1}{2} * \sum_{m,n,k} \Big\{ (\nu_v)'_{m,n}\ frvwl_{m,n} + (\nu_v)'_{m+1,n}\ frvwl_{m+1,n} +$$

$$(\nu_v)_{m,n}\ frvwl_{m,n} + (\nu_v)_{m+1,n}\ frvwl_{m+1,n} +$$

$$\frac{(\nu_\zeta)_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} \left(\frac{u'_{m,n} E_{m,n}}{\Delta\xi} \right) + \frac{(\nu_\zeta)_{m+1,n}}{K^\eta_{m+1,n} E^\xi_{m+1,n}} \left(\frac{-u'_{m,n} E_{m,n}}{\Delta\xi} \right) +$$

$$\frac{(\nu_\zeta)_{m+1,n+1}}{K^\eta_{m+1,n+1} E^\xi_{m+1,n+1}} \left(\frac{-u'_{m,n+1} E_{m,n+1}}{\Delta\xi} \right) +$$

$$\frac{(\nu_\zeta)_{m,n+1}}{K^\eta_{m,n+1} E^\xi_{m,n+1}} \left(\frac{u'_{m,n+1} E_{m,n+1}}{\Delta\xi} \right) +$$

$$\frac{(\nu_\zeta)_{m,n}}{K^\eta_{m,n} E^\xi_{m,n}} \left(\frac{v_{m,n} K_{m,n}}{\Delta\eta} \right) + \frac{(\nu_\zeta)_{m+1,n}}{K^\eta_{m+1,n} E^\xi_{m+1,n}} \left(\frac{v_{m+1,n} K_{m+1,n}}{\Delta\eta} \right) +$$

$$\frac{(\nu_\zeta)_{m+1,n+1}}{K^\eta_{m+1,n+1} E^\xi_{m+1,n+1}} \left(\frac{-v_{m+1,n} K_{m+1,n}}{\Delta\eta} \right) + \frac{(\nu_\zeta)_{m,n+1}}{K^\eta_{m,n+1} E^\xi_{m,n+1}} \left(\frac{-v_{m,n} K_{m,n}}{\Delta\eta} \right) \Big\}$$

The gradient for depth is calculated in WAQAD module AD-GRDP.

3.4.3. Boundary conditions

In this subsection the expression of the gradient for the boundary condition is derived. The parameters to be estimated are correction factors for the amplitude and phase of the boundary condition in point (m,n).

An overview of the contributions of the WAQUA continuity and momentum equations was given in section 3.2.3. The only terms containing the boundary condition parameters are:

$$(\nu_\zeta)_{m,n} \{ \Delta\zeta_{m,n} - \Delta A \cos(\omega t - \phi) - A \sin(\omega t - \phi) \Delta\phi \}$$

$$(\nu_\zeta)'_{m,n} \{ \Delta\zeta'_{m,n} - \Delta A \cos(\omega(t + \tfrac{1}{2}\Delta t) - \phi) - A \sin(\omega(t + \tfrac{1}{2}\Delta t) - \phi) \Delta\phi \}$$

The expression for the gradient of the amplitude and phase at the first stage becomes:

$$\frac{\partial J}{\partial A} = - (\nu_\zeta)'_{m,n} \cos(\omega(t + \tfrac{1}{2}\Delta t) - \phi)$$

$$\frac{\partial J}{\partial \phi} = - (\nu_\zeta)'_{m,n} A \sin(\omega(t + \tfrac{1}{2}\Delta t) - \phi)$$

And the expression for the gradient of the amplitude and phase at the second stage becomes:

$$\frac{\partial J}{\partial A} = - (\nu_\zeta)_{m,n} \cos(\omega t - \phi)$$

$$\frac{\partial J}{\partial \phi} = - (\nu_\zeta)_{m,n} A \sin(\omega t - \phi)$$

In WAQAD module AD-GRKB the boundary conditions (described by section 3.2.2) are solved first. Then the gradient for the amplitude and phase is calculated.

3.5. Remarks on WAQAD with respect to WAQUA

The remarks on WAQAD with respect to WAQUA are:

- The WAQAD bottom friction terms fruu, fruv, fruwl described by equation (3.14) and the terms frvu, frvv, frvwl described by equation (3.11) contain a shift of half a time step compared with the bottom friction terms in WAQUA.

- The horizontal advection terms are solved in WAQUA using the Gauss-Seidel method. In WAQAD these horizontal advection terms are solved using a Jacobi method.

- Horizontal viscosity is not included in WAQAD, but it is in WAQUA.

- Additional features of WAQUA which are not mentioned in [Stelling, 1984] are not included in WAQAD. This may lead to problems. For example:
  - External forcings, apart from open boundary values. Forcings like wind, discharges and density gradient influence the results of the WAQUA computations. WAQAD does not take these influences into account, which may lead to an unreliable gradient.
  - Transports, STRESS2d, barriers and weirs are taken into account by WAQUA, but not by WAQAD.
  - Smoothing boundary values.
    WAQUA has the option to smooth the boundary values during the play-in period. This option is not supported by WAQAD.
  - Depth multiplier.
    In the simulation input file a depth multiplier can be specified, which causes the depth values to be modified. When calibrating depth parameters, this option will definitely lead to erroneous results!! WAQAD has no knowledge of this multiplier and will deliver WAQUA adapted depth values as if the depth multiplier is 1.

- WAQUA writes map data only at every whole time step and not at every half time step. In WAQAD the map data at whole time steps is interpolated to half time steps.

4. The 3D adjoint model

This chapter goes into the adjoint model for three dimensional shallow water flow in detail. The adjoint model equations are derived in section 4.4. The adjoint solver as it is implemented in WAQAD is discussed in section 4.3. The derivation of the gradient is given in section 4.4. An overview of the remarks on WAQAD with respect to TRIWAQ is shown in section 4.5.

4.1. Introduction

One major shortcoming of the two dimensional shallow water flow model (WAQUA) is the fundamental loss of information about vertical structures of velocities. This property is inherent in the 2D depth averaged shallow water equations. The first three-dimensional model used at Rijkswaterstaat was proposed by [Leendertse, 1989]. It used a rectangular grid in both horizontal and vertical planes. Stelling also proposed a three-dimensional model based on so-called sigma coordinates. In 1992 Rijkswaterstaat/RIKZ built a three-dimensional system (TRIWAQ) with curvilinear coordinates in the horizontal plane and a general description of layer interfaces in the vertical plane. This prescription can be made by defining the layer thickness either relatively or absolutely in relation to the total water depth. For an extended description of this three- dimensional shallow water flow model, see the technical documentation of TRIWAQ, [Lander et al., 1996].

The adjoint model for the simplified three-dimensional shallow water equations was derived by [Mouthaan, 1995] in order to calibrate TRIWAQ. This chapter describes the 3D adjoint model as it is implemented in the current version of WAQAD: version 2.1, see the WAQAD User's Guide [Brouwer, 1996b] and the System Documentation of WAQAD [Brouwer, 1996a]. For more information on the implementation, see [Rozendaal, 1996].

4.2. The adjoint model equations

In this section the adjoint model for a simplified three-dimensional hydrodynamic sea model will be presented. The adjoint equations were derived using the Chavent method outlined in chapter 2. But before presenting these, the hydrodynamics of the forward model are described.

As in the case of the 2D model, the mathematical description of three-dimensional water flow consists of a system of coupled differential equations which are physically based on the laws for the conservation of mass and momentum, deduced from the Navier Stokes equations. The simplified, i.e. advection and horizontal viscosity are ignored, three-dimensional hydrodynamic equations for continuity and motion may be written in Cartesian coordinates as, [De Goede, 1992]:

$$\frac{\partial u}{\partial t} = f\ v - g\ \frac{\partial \zeta}{\partial x} + \frac{\partial}{\partial z}\left(\nu_v \frac{\partial u}{\partial z} \right)$$

$$\frac{\partial v}{\partial t} = -\ f\ u - g\ \frac{\partial \zeta}{\partial y} + \frac{\partial}{\partial z}\left(\nu_v \frac{\partial v}{\partial z} \right)$$

$$\frac{\partial \zeta}{\partial t} = -\ \frac{\partial}{\partial x}\left(\int_{-d}^{\zeta} u\, \partial z \right) - \frac{\partial}{\partial y}\left(\int_{-d}^{\zeta} v\, \partial z \right)$$

in which:

u, v	=	Velocity components in x and y directions
ζ	=	Water elevation above plane of reference
f	=	Coriolis coefficient
g	=	Acceleration of gravity
ν_v	=	Vertical viscosity coefficient

The two-stage time splitting method (ADI), as used in the 2D model, is used to integrate the model equations of the three-dimensional shallow water flow model. However, a slightly different approach is used for the vertical viscosity terms: they are always taken implicitly in time. Because the coefficients vary in time in the vertical terms, the unconditional stability cannot be reached with central time derivatives [Lander et al., 1996].

The discretized equations in space and time for the simplified three-dimensional hydrodynamic model are the starting point for the deduction of the corresponding adjoint equations. Since the two stages of a time step are virtually identical, only

one stage will be considered. For an interior point in the field not enclosed by impeded geometry the flow is described by:

Conservation of momentum per layer in y direction in the first stage:

$$\frac{[\,v' - v\,]}{\frac{1}{2}\,\Delta t} + \overline{f\,u}^{\,\xi\eta} + \frac{g}{E^{v}}\,\zeta_{0\eta} = \delta_z\left(\,\nu_V\,\delta_z\,v'\,\right) \tag{4.1}$$

The vertically integrated continuity equation in the first stage:

$$\frac{[\,\zeta' - \zeta\,]}{\frac{1}{2}\,\Delta t} = -\,\frac{(H\,U\,E)'_{o\xi} + (\,H\,V\,K\,)_{0\eta}}{K^{\eta}\,E^{\xi}} \tag{4.2}$$

Conservation of momentum per layer in x direction in the first stage:

$$\frac{[\,u' - u\,]}{\frac{1}{2}\,\Delta t} - \overline{f\,v'}^{\,\eta\xi} + \frac{g}{K^{u}}\,\zeta'_{0\xi} = \delta_z\left(\,\nu_V\,\delta_z\,u'\,\right) \tag{4.3}$$

in which:

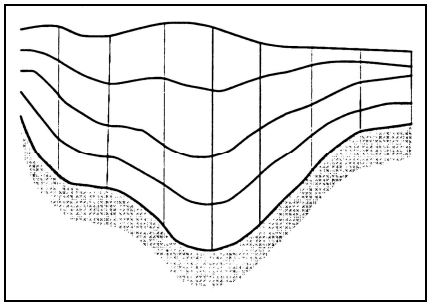
H	=	Total water depth
U	=	Depth-averaged horizontal velocity component in x direction
V	=	Depth-averaged horizontal velocity component in y direction
ξ, η	=	Horizontal curvilinear coordinates
K	=	gvv, the WAQUA transformation coefficient in ξ direction, see subsection 3.2.1
E	=	guu, the WAQUA transformation coefficient in η direction, see subsection 3.2.1
h	=	Layer thickness at u point, also denoted as hu
h^{v}	=	Layer thickness at v point
k	=	Layer index
K	=	Number of layers
z_k	=	Position of layer interface
Δt	=	Integration time step

Remarks:

- The state in the new time level t+½Δt is denoted by a single apostrophe. The absence of an apostrophe indicates the state in time level t. For convenience, only indices which deviate from m, n, k are denoted. The terms considered in these forward model equations do not

require a special boundary treatment. Therefore, the corresponding adjoint equations do not change near boundaries.

- In the TRIWAQ system a grid definition in the vertical plane needing the prescription of K+1 layer interfaces z_K is used. The layer thickness h_K is defined as $z_{K-1} - z_K$. Notice that z_0 equals the water level ζ and z_K equals the bottom with opposite sign. The sigma coordinates σ are obtained using the following transformation:



$$1\sigma = \frac{z - \zeta}{H}, \quad \sigma \in [-1, 0]$$

figure 4.1 Sigma transformation

The layer thickness is defined in a relative way as a constant part of the total water depth. However, it is also possible to use layer thicknesses defined in an absolute way.

The Chavent method as described in chapter 2 is applied to these forward model equations (4.1 - 4.3) to obtain the corresponding adjoint equations. Since the derivation has already been described in detail for the two-dimensional case in chapter 3, the derivation for the three-dimensional case is omitted here. The results of the derivation are summarized:

Adjoint conservation of mass in the first stage:

$$\frac{\left[(\nu_\zeta)' - (\nu_\zeta)''\right]}{\frac{1}{2}\,\Delta t} - g\left(\frac{\sum_k (\nu_u)' + \sum_k (\nu_u)''}{K^u}\right)_{0\xi} \tag{4.4}$$

$$-\overline{\left[U'\,E\left(\frac{(\nu_\zeta)' + (\nu_\zeta)''}{K^\eta\,E^\xi}\right)_{0\xi}\right]}^{\xi}$$

$$+\overline{\left[\sum_{k=2}^{K}\left[\sigma_{k-2} - \sigma_{k-1}\right](\nu_u)''_k\,\frac{\overline{\nu_v}^{\xi}\left(u''_{k-1} - u''\right)}{\frac{1}{2}\,h'\left(h'_{k-1} + h'\right)^2}\right]}^{\xi}$$

$$+\overline{\left[\sum_{k=2}^{K}\left[\sigma_{k-1} - \sigma_k\right](\nu_u)''_k\,\frac{\overline{\nu_v}^{\xi}\left(u''_{k-1} - u''\right)\left(h'_{k-1} + 2h'\right)}{\frac{1}{2}\left(h'\right)^2\left(h'_{k-1} + h'\right)^2}\right]}^{\xi}$$

$$-\overline{\left[\sum_{k=1}^{K-1}\left[\sigma_{k-1} - \sigma_k\right](\nu_u)''_k\,\frac{\overline{\nu_v}^{\xi}\left(u'' - u''_{k+1}\right)\left(2h' + h'_{k+1}\right)}{\frac{1}{2}\left(h'\right)^2\left(h' + h'_{k+1}\right)^2}\right]}^{\xi}$$

$$-\overline{\left[\sum_{k=1}^{K-1}\left[\sigma_k - \sigma_{k+1}\right](\nu_u)''_k\,\frac{\overline{\nu_v}^{\xi}\left(u'' - u''_{k+1}\right)}{\frac{1}{2}\,h'\left(h' + h'_{k+1}\right)^2}\right]}^{\xi}$$

$$+\overline{\left[\sum_{k=2}^{K}\left[\sigma_{k-2} - \sigma_{k-1}\right](\nu_v)''_k\,\frac{\overline{\nu_v}^{\eta}\left(v''_{k-1} - v''\right)}{\frac{1}{2}\,h'^{,v}\left(h'^{,v}_{k-1} + h'^{,v}\right)^2}\right]}^{\eta}$$

$$+\overline{\left[\sum_{k=2}^{K}\left[\sigma_{k-1} - \sigma_k\right](\nu_v)''_k\,\frac{\overline{\nu_v}^{\eta}\left(v''_{k-1} - v''\right)\left(h'^{,v}_{k-1} + 2h'^{,v}\right)}{\frac{1}{2}\left(h'^{,v}\right)^2\left(h'^{,v}_{k-1} + h'^{,v}\right)^2}\right]}^{\eta}$$

$$-\overline{\left[\sum_{k=1}^{K-1}\left[\sigma_{k-1} - \sigma_k\right](\nu_v)''_k\,\frac{\overline{\nu_v}^{\eta}\left(v'' - v''_{k+1}\right)\left(2h'^{,v} + h'^{,v}_{k+1}\right)}{\frac{1}{2}\left(h'^{,v}\right)^2\left(h'^{,v} + h'^{,v}_{k+1}\right)^2}\right]}^{\eta}$$

$$-\overline{\left[\sum_{k=1}^{K-1}\left[\sigma_k - \sigma_{k+1}\right](\nu_v)''_k\,\frac{\overline{\nu_v}^{\eta}\left(v'' - v''_{k+1}\right)}{\frac{1}{2}\,h'^{,v}\left(h'^{,v} + h'^{,v}_{k+1}\right)^2}\right]}^{\eta}$$

$$-\overline{\left[\left[\sigma_{K-1} - \sigma_K\right](\nu_u)''_k\,\frac{g}{C^2}\,\frac{u''_K\sqrt{\left(u'_K\right)^2 + \left(\overline{v'_K}^{\eta\xi}\right)^2}}{\left(h'_K\right)^2}\right]}^{\xi}$$

$$-\overline{\left[\left[\sigma_{K-1} - \sigma_K\right](\nu_v)''_K\,\frac{g}{C^2}\,\frac{v''_K\sqrt{\left(v'_K\right)^2 + \left(\overline{u''_K}^{\xi\eta}\right)^2}}{\left(h'^{,v}_K\right)^2}\right]}^{\eta} = 0$$

Adjoint conservation of momentum in x direction per layer in the first stage:

$$\frac{[(\nu_u)' - (\nu_u)'']}{\frac{1}{2}\Delta t} - h' E\left(\frac{(\nu_\zeta)' + (\nu_\zeta)''}{K^\eta E^\xi} \right)_{0\xi}$$
$$- \frac{\overline{\nu_v}^{\,\xi}}{\frac{1}{2}(h_{k-1} + h)} \left[\frac{(\nu_u)'_{k-1}}{h_{k-1}} - \frac{(\nu_u)'}{h} \right] \qquad (4.5)$$
$$+ \frac{\overline{\nu_v}^{\,\xi}}{\frac{1}{2}(h + h_{k+1})} \left[\frac{(\nu_u)'}{h} - \frac{(\nu_u)'_{k+1}}{h_{k+1}} \right] = 0$$

Adjoint conservation of momentum in y direction per layer in the first stage:

$$\frac{[(\nu_v)' - (\nu_v)'']}{\frac{1}{2}\Delta t} - \left[\overline{f(\nu_u)'}^{\,\xi\eta} + \overline{f(\nu_u)''}^{\,\xi\eta} \right]$$
$$- \frac{\overline{\nu_v}^{\,\eta}}{\frac{1}{2}\left(h^v_{k-1} + h^v\right)} \left[\frac{(\nu_v)'_{k-1}}{h^v_{k-1}} - \frac{(\nu_v)'}{h^v} \right] \qquad (4.6)$$
$$+ \frac{\overline{\nu_v}^{\,\eta}}{\frac{1}{2}\left(h^v + h^v_{k+1}\right)} \left[\frac{(\nu_v)'}{h^v} - \frac{(\nu_v)'_{k+1}}{h^v_{k+1}} \right] = 0$$

in which:

(ν_ζ) = adjoint water level
(ν_u) = adjoint velocity in x direction for a layer
(ν_v) = adjoint velocity in y direction for a layer

Remarks:

- Note that the vertical viscosity coefficient and the adjoint velocity in y direction are denoted by the same symbol ν_v. However, the adjoint velocity in y direction is marked by braces: (ν_v).

- The adjoint equations in the second stage are virtually identical and can easily be deduced from the ones in the first stage by [Stelling, 1984]:
  - the interchange of ξ and η , u and v
  - the alteration of sign of the Coriolis coefficient
  - the transformation of the time level with half a timestep

- The adjoint equations for the simplified three-dimensional shallow water equations are deduced with the Chavent method. Since uncertain boundaries are not prescribed, homogeneous boundary conditions for the adjoint model

are assumed. Therefore, calibration of boundary condition parameters is not implemented in WAQAD in the case of three-dimensional models.

- WAQAD takes account of dryfall in the case of three-dimensional models in the same way as in the case of two dimensional models. The adjoint drying and flooding procedure, described in subsection 3.2.4, is also applied to the 3D adjoint model equations.

- The adjoint model is activated by the misfits between the observed data and the corresponding model values. Residuals of observed and computed water levels affect the adjoint continuity equation. If a water level measurement has been recorded at full time levels, the residual has to be added to the right-hand side of the corresponding adjoint continuity equation in the second stage.

- Differentials of layer thicknesses were transcribed into differentials of water levels. Since $h_k = z_{k-1} - z_k$ and $z_k = \sigma_k \; H + \zeta$, it follows that $\Delta h_k = \frac{1}{2} \; (\sigma_{k-1} - \sigma_k) \; (\Delta \zeta_m + \Delta \zeta_{m+1})$. It is assumed that no fixed layers are prescribed in the forward model.

- A central time integration of the vertical terms in the momentum equations of the forward model is assumed. Since it is possible for the approximation of the vertical viscosity to be fully implicit, the Euler implicit variant has in fact become redundant.

- There are several options to define the vertical viscosity coefficient in TRIWAQ: by means of a constant value, the algebraic model or the k-eps model (see the WAQUA User's Guide). WAQAD can estimate the vertical viscosity parameters for all the options mentioned.

4.3. The adjoint solver

This section deals with the method for solving the adjoint equations deduced from the Chavent method for the simplified three-dimensional shallow water flow model. This solution method also has a two-stage time-splitting structure. However, only the first stage is considered, since the other stage is virtually identical, due to the underlying ADI method, [Stelling, 1984]. Similar to the approach in the forward model, the approximation of the vertical viscosity terms in the adjoint momentum equations is fully implicit. For detailed information on the numerical treatment of the discretized equations in the forward model, see [Lander et al., 1996].

The inverse model equations are solved in reverse order compared with the three-dimensional shallow water flow model. In the first stage in WAQAD the adjoint continuity equation and the adjoint u momentum equation are solved in module AD-SUV3 first and then the adjoint v momentum equation is solved in module AD-VYD3. In the second stage in WAQAD the adjoint continuity equation and the adjoint v momentum equation are solved in module AD-SVU3 first and then the adjoint u momentum equation is solved in module AD-UXD3.

Below, the modules of the first stage are discussed: AD-SUV3 and AD-VYD3.

AD-SUV3

The adjoint conservation of mass appears to be a pentadiagonal matrix equation. Combined with the adjoint u momentum equation a tridiagonal system in adjoint water levels is obtained, which can easily be solved, and afterwards the adjoint u velocities can be determined.

The starting point of the description of the solution method is that the adjoint conservation of momentum per layer in x direction (4.5) can be written in the following form:

$$a_{m,k}\ \frac{(\nu_\zeta)'_m}{K^{\eta}\ E^{\xi}} + b_{m,k}\ (\nu_u)'_{m,k} + c_{m,k}\ \frac{(\nu_\zeta)'_{m+1}}{K^{\eta}_{m+1}\ E^{\xi}_{m+1}} + e_{m,k}\ (\nu_u)'_{m,k-1} + f_{m,k}\ (\nu_u)'_{m,k+1} = d_{m,k} \tag{4.7}$$

in which:

$$a_{m,k} = \frac{h'\ E}{\Delta\xi}$$

$$b_{m,k} = \frac{1}{\tfrac{1}{2}\ \Delta t} + \frac{\overline{\nu_v}^{\xi}}{\tfrac{1}{2}\ h\ (\ h_{k-1} + h\ )} + \frac{\overline{\nu_v}^{\xi}}{\tfrac{1}{2}\ h\ (h + h_{k+1})}$$

$$c_{m,k} = -\frac{h'\ E}{\Delta\xi}$$

$$e_{m,k} = -\ \frac{\overline{\nu_v}^{\xi}}{\tfrac{1}{2}\ h_{k-1}\ (\ h_{k-1} + h\ )}$$

$$f_{m,k} = -\ \frac{\overline{\nu_v}^{\xi}}{\tfrac{1}{2}\ h_{k+1}\ (\ h + h_{k+1}\ )}$$

$$d_{m,k} = \frac{(\nu_u)''}{\tfrac{1}{2}\ \Delta t} + h'\ E\left(\ \frac{(\nu_\zeta)''}{K^{\eta}\ E^{\xi}}\ \right)_{0\xi}$$

The layer thicknesses can be calculated from the total water depth and the sigma coordinates.

In more compact form:

$$A\ \underline{(\nu_u)'} = \underline{d} - \frac{(\nu_\zeta)'_m}{K^{\eta}\ E^{\xi}}\ \underline{a} - \frac{(\nu_\zeta)'_{m+1}}{K^{\eta}_{m+1}\ E^{\xi}_{m+1}}\ \underline{c} \qquad (4.8)$$

in which:

$$\underline{(\nu_u)'} = \left[\ (\nu_u)'_1\ ,\ (\nu_u)'_2\ ,\ \cdots\ ,\ (\nu_u)'_K\ \right]^T$$

$$\underline{d} = \left[\ d_1\ ,\ d_2\ ,\ \cdots\ ,\ d_K\ \right]^T$$

$$\underline{a} = \left[\ a_1\ ,\ a_2\ ,\ \cdots\ ,\ a_K\ \right]^T$$

$$\underline{c} = \left[\ c_1\ ,\ c_2\ ,\ \cdots\ ,\ c_K\ \right]^T$$

and

$$A = \begin{bmatrix} b_{m,1} & f_{m,1} & & & \\ e_{m,2} & b_{m,2} & f_{m,2} & & \\ & \cdots & \cdots & \cdots & \\ & & \cdots & \cdots & \cdots \\ & & & e_{m,K} & b_{m,K} \end{bmatrix}$$

$$f_{m,1} = -\ \frac{\overline{\nu_v}^{\xi}}{\tfrac{1}{2}\ h_2\ (\ h_1 + h_2\ )}$$

$$e_{m,K} = -\ \frac{\overline{\nu_v}^{\xi}}{\tfrac{1}{2}\ h_{K-1}\ (\ h_{K-1} + h\ )}$$

In the uppermost layer a term associated with wind stress is defined, however, the wind stress in WAQAD is supposed to be equal to zero. In the lowermost layer a term associated with bottom roughnouss is defined; the two-dimensional approach is used for the adjoint momentum equations in the bottom layer. Here, on the main diagonal, part of the vertical viscosity term still remains.

The right-hand side of this equation (4.8) is independent of $\underline{(\nu_u)'}$, so the tridiagonal matrix A can be inverted, which formally leads to:

$$\frac{(\nu_\zeta)'_m}{K^{\eta}\ E^{\xi}}\ A^{-1}\ \underline{a} + \underline{(\nu_u)'} + \frac{(\nu_\zeta)'_{m+1}}{K^{\eta}_{m+1}\ E^{\xi}_{m+1}}\ A^{-1}\ \underline{c} = A^{-1}\ \underline{d} \qquad (4.9)$$

In practice it is not necesary to compute the whole matrix A^{-1}: the three tridiagonal systems can be solved by a double sweep. This strategy decouples the adjoint u velocity points in the vertical. Using equation (4.9) again, the momentum equation per layer can be derived:

$$(\mathrm{AAK})_{m,k}\,\frac{(\nu_\zeta)'_m}{K^{\eta}\,E^{\xi}} + (\nu_u)'_{m,k} + (\mathrm{CCK})_{m,k}\,\frac{(\nu_\zeta)'_{m+1}}{K^{\eta}_{m+1}\,E^{\xi}_{m+1}} = (\mathrm{DDK})_{m,k} \qquad (4.10)$$

in which:

$(\mathrm{AAK})_{m,k}$ = k-th element of A^{-1} $\underline{a}$
$(\mathrm{CCK})_{m,k}$ = k-th element of A^{-1} $\underline{c}$
$(\mathrm{DDK})_{m,k}$ = k-th element of A^{-1} $\underline{d}$

These equations have to be added up per layer from bottom to top in order to eliminate the adjoint u velocities at the implicit time level in the adjoint continuity equation. The vertically summed adjoint u momentum equation is then:

$$\frac{(\nu_\zeta)'_m}{K^{\eta}\,E^{\xi}}\sum_k(\mathrm{AAK})_{m,k} + \sum_k(\nu_u)'_{m,k} + \frac{(\nu_\zeta)'_{m+1}}{K^{\eta}_{m+1}\,E^{\xi}_{m+1}}\sum_k(\mathrm{CCK})_{m,k} = \sum_k(\mathrm{DDK})_{m,k} \qquad (4.11)$$

which will be noted as:

$$(\mathrm{AA})_m\,\frac{(\nu_\zeta)'_m}{K^{\eta}\,E^{\xi}} + \sum_k(\nu_u)'_{m,k} + (\mathrm{CC})_m\,\frac{(\nu_\zeta)'_{m+1}}{K^{\eta}_{m+1}\,E^{\xi}_{m+1}} = (\mathrm{DD})_m \qquad (4.12)$$

in which:

$$(\mathrm{AA})_m = \sum_k(\mathrm{AAK})_{m,k}$$
$$(\mathrm{CC})_m = \sum_k(\mathrm{CCK})_{m,k}$$
$$(\mathrm{DD})_m = \sum_k(\mathrm{DDK})_{m,k}$$

After eliminating the adjoint u velocities from their adjoint momentum equations (4.12) in the adjoint conservation of mass (4.4), a tridiagonal system in adjoint water levels is formed, which can be resolved by the well known double sweep method, [Stelling, 1984]:

$$A_m \ (\nu_\zeta)'_{m-1} + B_m \ (\nu_\zeta)'_m + C_m \ (\nu_\zeta)'_{m+1} = D_m \qquad (4.13)$$

in which:

$$A_m = \frac{1}{K^{\eta}_{m-1} \ E^{\xi}_{m-1}} \left\{ \frac{u'_{m-1} \ E_{m-1}}{2 \ \Delta\xi} - \frac{g \ (\ AA \ )_{m-1}}{K^{u}_{m-1} \ \Delta\xi} \right\}$$

$$B_m = \frac{1}{\frac{1}{2} \ \Delta t} + \frac{1}{K^{\eta} \ E^{\xi}} \left\{ \frac{1}{2} \ (\ U' E \ )_{0\xi} - \frac{g \ (\ CC \ )_{m-1}}{K^{u} \ \Delta\xi} + \frac{g \ (\ AA \ )_m}{K^{u} \ \Delta\xi} \right\}$$

$$C_m = \frac{1}{K^{\eta}_{m+1} \ E^{\xi}_{m+1}} \left\{ - \frac{U' E}{2 \ \Delta\xi} + \frac{g \ (\ CC \ )_m}{K^{u} \ \Delta\xi} \right\}$$

and:

$$
\begin{aligned}
D_m = \frac{(\nu_\zeta)''}{\tfrac{1}{2}\,\Delta t} + g\left(\frac{\sum_k (\nu_u)'' + (\,DD\,)_m}{K^u}\right)_{0\xi} + \overline{\left[U' E\left(\frac{(\nu_\zeta)''}{K^{\eta}\,E^{\xi}}\right)_{0\xi}\right]}^{\xi} \\
- \left[\overline{\sum_{k=2}^{K}[\sigma_{k-2}-\sigma_{k-1}](\nu_u)''_k \frac{\overline{\nu_v}^{\xi}(u''_{k-1}-u'')}{\tfrac{1}{2}h'(h'_{k-1}+h')^2}}\right]^{\xi} \\
- \left[\overline{\sum_{k=2}^{K}[\sigma_{k-1}-\sigma_k](\nu_u)''_k \frac{\overline{\nu_v}^{\xi}(u''_{k-1}-u'')(h'_{k-1}+2h')}{\tfrac{1}{2}(h')^2(h'_{k-1}+h')^2}}\right]^{\xi} \\
+ \left[\overline{\sum_{k=2}^{K-1}[\sigma_{k-1}-\sigma_k](\nu_u)''_k \frac{\overline{\nu_v}^{\xi}(u''-u''_{k+1})(2h'+h'_{k+1})}{\tfrac{1}{2}(h')^2(h'+h'_{k+1})^2}}\right]^{\xi} \\
+ \left[\overline{\sum_{k=1}^{K-1}[\sigma_k-\sigma_{k+1}](\nu_u)''_k \frac{\overline{\nu_v}^{\xi}(u''-u''_{k+1})}{\tfrac{1}{2}h'(h'+h'_{k+1})^2}}\right]^{\xi} \\
- \left[\overline{\sum_{k=2}^{K}[\sigma_{k-2}-\sigma_{k-1}](\nu_v)''_k \frac{\overline{\nu_v}^{\eta}(v''_{k-1}-v'')}{\tfrac{1}{2}h'^{,v}(h'^{,v}_{k-1}+h'^{,v})^2}}\right]^{\eta} \\
- \left[\overline{\sum_{k=2}^{K}[\sigma_{k-1}-\sigma_k](\nu_v)''_k \frac{\overline{\nu_v}^{\eta}(v''_{k-1}-v'')(h'^{,v}_{k-1}+2h'^{,v})}{\tfrac{1}{2}(h'^{,v})^2(h'^{,v}_{k-1}+h'^{,v})^2}}\right]^{\eta} \\
+ \left[\overline{\sum_{k=1}^{K-1}[\sigma_{k-1}-\sigma_k](\nu_v)''_k \frac{\overline{\nu_v}^{\eta}(v''-v''_{k+1})(2h'^{,v}+h'^{,v}_{k+1})}{\tfrac{1}{2}(h'^{,v})^2(h'^{,v}+h'^{,v}_{k+1})^2}}\right]^{\eta} \\
+ \left[\overline{\sum_{k=1}^{K-1}[\sigma_k-\sigma_{k+1}](\nu_v)''_k \frac{\overline{\nu_v}^{\eta}(v''-v''_{k+1})}{\tfrac{1}{2}h'^{,v}(h'^{,v}+h'^{,v}_{k+1})^2}}\right]^{\eta} \\
+ \left[\overline{[\sigma_{K-1}-\sigma_K](\nu_u)''_K \frac{g}{C^2}\frac{u''_K\sqrt{(u'_K)^2+\left(\overline{v'_K}^{\eta\xi}\right)^2}}{(h'_K)^2}}\right]^{\xi} \\
+ \left[\overline{[\sigma_{K-1}-\sigma_K](\nu_v)''_K \frac{g}{C^2}\frac{v''_K\sqrt{(v'_K)^2+\left(\overline{u'_K}^{\eta\xi}\right)^2}}{(h'^{,v}_K)^2}}\right]^{\eta}
\end{aligned}
$$

Now $(\nu_\zeta)'_m$ can be solved, and thereafter $(\nu_u)'_{m,k}$ can be computed per layer with the adjoint u momentum equation. Note that the bottom roughness formulation equals its two-dimensional version.

AD-VYD3

The adjoint conservation of momentum per layer in y direction in the first stage (4.6) can be written in the following form:

$$a_k\ (\nu_v)'_{k-1} + b_k\ (\nu_v)'_k + c_k\ (\nu_v)'_{k+1} = d_k \tag{4.14}$$

in which:

$$a_k = -\ \frac{\overline{\nu_v}^{\eta}}{\tfrac{1}{2}\ h^v_{k-1}\left(\ h^v_{k-1} + h^v\ \right)}$$

$$b_k = \frac{1}{\tfrac{1}{2}\ \Delta t} + \frac{\overline{\nu_v}^{\eta}}{\tfrac{1}{2}\ h^v\left(\ h^v_{k-1} + h^v\ \right)} + \frac{\overline{\nu_v}^{\eta}}{\tfrac{1}{2}\ h^v\left(\ h^v + h^v_{k+1}\ \right)}$$

$$c_k = -\ \frac{\overline{\nu_v}^{\eta}}{\tfrac{1}{2}\ h^v_{k+1}\left(\ h^v + h^v_{k+1}\ \right)}$$

$$d_k = \frac{(\nu_v)''}{\tfrac{1}{2}\ \Delta t} + \left[\ \overline{f\,(\nu_u)'}^{\xi\eta} + \overline{f\,(\nu_u)''}^{\xi\eta}\ \right]$$

In more compact form:

$$A\ \underline{(\nu_v)'} = \underline{d} \tag{4.15}$$

in which:

$$\underline{(\nu_v)'} = \left[\ (\nu_v)'_1\ ,\ (\nu_v)'_2\ ,\ \cdots\ ,\ (\nu_v)'_K\ \right]^T$$

$$\underline{d} = \left[\ d_1\ ,\ d_2\ ,\ \cdots\ ,\ d_K\ \right]^T$$

and

$$A = \begin{bmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \cdots & \cdots & \cdots & \\ & & \cdots & \cdots & \cdots \\ & & & a_k & b_k \end{bmatrix}$$

$$c_1 = -\ \frac{\overline{\nu_v}^{\eta}}{\tfrac{1}{2}\ h^v_2\left(\ h^v_1 + h^v_2\ \right)}$$

$$a_K = -\ \frac{\overline{\nu_v}^{\eta}}{\tfrac{1}{2}\ h^v_{K-1}\left(\ h^v_{K-1} + h^v\ \right)}$$

This tridiagonal system in adjoint v velocities can be solved by the well known double sweep method. For this, the layer thicknesses are determined from the computed total water depth and the sigma coordinates, and at the exterior layers a term associated with wind stress or bottom roughness is also defined. The two-dimensional approach is used here. Part of the vertical viscosity term still remains on the main diagonal associated with these layers.

Remarks:

- Since no uncertain boundary conditions are assumed, it is not necessary to solve the adjoint boundary conditions. Therefore, calibrating boundary condition by using 3D adjoint is not implemented in WAQAD.

- The drying and flooding procedure in the 3D case is implemented in WAQAD in the same way as in the 2D case. This procedure is implemented in the 3D modules AD-SUV3, AD-SVU3, AD-VYD3 and AD-UXD3 according to subsection 3.3.3.

- In the lowermost layer of the 3D model bottom roughness is assumed. The same approach is applied to the 3D case as in the 2D case. This means that the bottom friction terms for the 3D model are calculated in the same way as for the 2D model. The bottom friction contributions to the u and v momentum equations are calculated in a similar way by equations (3.11) and (3.14):

$$fruu^{3d} = \frac{g}{C_u^2} \frac{2(u_K)^2 + (\overline{v_K}^{\eta\xi})^2}{h_K \sqrt{(u_K)^2 + (\overline{v_K}^{\eta\xi})^2}}$$

$$fruv^{3d} = \frac{g}{C_u^2} \frac{u_K \overline{v_K}^{\eta\xi}}{h_K \sqrt{(u_K)^2 + (\overline{v_K}^{\eta\xi})^2}}$$

$$frvu^{3d} = \frac{g}{C_v^2} \frac{\overline{u_K}^{\xi\eta} v_K}{h_K^v \sqrt{(\overline{u_K}^{\xi\eta})^2 + (v_K)^2}}$$

$$frvv^{3d} = \frac{g}{C_v^2} \frac{(\overline{u_K}^{\xi\eta})^2 + 2(v_K)^2}{h_K^v \sqrt{(\overline{u_K}^{\xi\eta})^2 + (v_K)^2}}$$

However, the bottom friction contribution to the adjoint continuity equation is calculated by the last two terms of coefficient D_m of equation (4.13):

$$frwl^{3d} = \frac{g}{C^2}\frac{u'_K\sqrt{(u'_K)^2 + \left(\overline{v_K}^{\eta\xi}\right)^2}}{(h_K)^2} + \frac{g}{C^2}\frac{v'_K\sqrt{(v_K)^2 + \left(\overline{u'_K}^{\xi\eta}\right)^2}}{(h_K^v)^2}$$

The term frwl is calculated at u points as well as v points every half time step. In the term frwl the shift of half a time step with respect to TRIWAQ is corrected.

4.4. The gradient

Once the adjoint state has been determined, the most difficult task of the inverse modeling technique has been accomplished. The gradient of the error function can now be computed easily with the adjoint solution.

In the following subsections the expression of the gradient is derived for the following three cases:

- the parameter to be estimated is a correction factor for the bottom friction coefficient, subsection 4.4.1.
- the parameter to be estimated is a correction factor for the depth, subsection 4.4.2.
- the parameter to be estimated is a correction factor for the vertical viscosity coefficient, subsection 4.4.3.

4.4.1. Bottom friction

The differential of an additive control parameter defined for Chezy in the first stage is given by:

$$-(\nu_v)''_K \frac{2g}{C^3} \frac{v''_K \sqrt{(v'_K)^2 + (\overline{u''_K}^{\xi\eta})^2}}{h'^v_K} - (\nu_u)''_K \frac{2g}{C^3} \frac{u_{K'} \sqrt{(u'_K)^2 + (\overline{v'_K}^{\eta\xi})^2}}{h'_K}$$

The differential of an additive control parameter defined for Chezy in the second stage is described by:

$$-(\nu_v)'_K \frac{2g}{C^3} \frac{v'_K \sqrt{(v_K)^2 + (\overline{u_k}^{\xi\eta})^2}}{h^v_K} - (\nu_u)'_k \frac{2g}{C^3} \frac{u'_K \sqrt{(u_K)^2 + (\overline{v'_K}^{\eta\xi})^2}}{h_K}$$

For bottom friction in case of Manning and White Colebrook, see section 5.6.

4.4.2. Depth

The differential of an additive control parameter defined for bathymetry in the first stage is given by:

$$-\overline{\left[U'E\left(\frac{(\nu_\zeta)''}{K^{\eta}E^{\xi}}\right)_{0\xi}\right]}^{\eta}-\overline{\left[V''K\left(\frac{(\nu_\zeta)''}{K^{\eta}E^{\xi}}\right)_{0\eta}\right]}^{\xi}$$

$$+\overline{\left[\sum_{k=2}^{K}[\sigma_{k-2}-\sigma_{k-1}](\nu_u)''\frac{\overline{\nu_v}^{\xi}(u''k-1-u'')}{\tfrac{1}{2}h'(h'_{k-1}+h')^2}\right]}^{\eta}$$

$$+\overline{\left[\sum_{k=2}^{K}[\sigma_{k-1}-\sigma_k](\nu_u)''\frac{\overline{\nu_v}^{\xi}(u''_{k-1}-u'')(h'_{k-1}+2h')}{\tfrac{1}{2}(h')^2(h'_{k-1}+h')^2}\right]}^{\eta}$$

$$-\overline{\left[\sum_{k=1}^{K-1}[\sigma_{k-1}-\sigma_k](\nu_u)''\frac{\overline{\nu_v}^{\xi}(u''-u''_{k+1})(2h'+h'_{k+1})}{\tfrac{1}{2}(h')^2(h'+h'_{k+1})^2}\right]}^{\eta}$$

$$-\overline{\left[\sum_{k=1}^{K-1}[\sigma_k-\sigma_{k+1}](\nu_u)''\frac{\overline{\nu_v}^{\xi}(u''-u''_{k+1})}{\tfrac{1}{2}h'(h'+h'_{k+1})^2}\right]}^{\eta}$$

$$+\overline{\left[\sum_{k=2}^{K}[\sigma_{k-2}-\sigma_{k-1}](\nu_v)''\frac{\overline{\nu_v}^{\eta}(v''_{k-1}-v'')}{\tfrac{1}{2}h'^{,v}(h'^{,v}_{k-1}+h'^{,v})^2}\right]}^{\xi}$$

$$+\overline{\left[\sum_{k=2}^{K}[\sigma_{k-1}-\sigma_k](\nu_v)''\frac{\overline{\nu_v}^{\eta}(v''_{k-1}-v'')(h'^{,v}_{k-1}+2h'^{,v})}{\tfrac{1}{2}(h'^{,v})^2(h'^{,v}_{k-1}+h'^{,v})^2}\right]}^{\xi}$$

$$-\overline{\left[\sum_{k=1}^{K-1}[\sigma_{k-1}-\sigma_k](\nu_v)''\frac{\overline{\nu_v}^{\eta}(v''-v''_{k+1})(2h'^{,v}+h'^{,v}_{k+1})}{\tfrac{1}{2}(h'^{,v})^2(h'^{,v}+h'^{,v}_{k+1})^2}\right]}^{\xi}$$

$$-\overline{\left[\sum_{k=1}^{K-1}[\sigma_k-\sigma_{k+1}](\nu_v)''\frac{\overline{\nu_v}^{\eta}(v''-v''_{k+1})}{\tfrac{1}{2}h'^{,v}(h'^{,v}+h'^{,v}_{k+1})^2}\right]}^{\xi}$$

$$-\overline{\left[\left[\sigma_{K-1}-\sigma_K\right](\nu_u)''_K\,\frac{g}{C^2}\,\frac{u''_K\sqrt{(u'_K)^2+(\overline{v'^{\eta\xi}_K})^2}}{(h'_K)^2}\right]}^{\eta}$$

$$-\overline{\left[\left[\sigma_{K-1}-\sigma_K\right](\nu_v)''_K\,\frac{g}{C^2}\,\frac{v''_K\sqrt{(v'_K)^2+(\overline{u''^{\xi\eta}_K})^2}}{(h'^{v}_K)^2}\right]}^{\xi}$$

The differential of an additive control parameter defined for bathymetry in the second stage is described by:

$$-\overline{\left[U'E\left(\frac{(\nu_\zeta)'}{K^{\eta}E^{\xi}}\right)_{0\xi}\right]}^{\eta}-\overline{\left[VK\left(\frac{(\nu_\zeta)'}{K^{\eta}E^{\xi}}\right)_{0\eta}\right]}^{\xi}$$

$$+\overline{\left[\sum_{k=2}^{K}[\sigma_{k-2}-\sigma_{k-1}](\nu_u)'\frac{\overline{\nu_v}^{\xi}(u'_{k-1}-u')}{\tfrac{1}{2}h(h_{k-1}+h)^2}\right]}^{\eta}$$

$$+\overline{\left[\sum_{k=2}^{K}[\sigma_{k-1}-\sigma_{k}](\nu_u)'\frac{\overline{\nu_v}^{\xi}(u'_{k-1}-u')(h_{k-1}+2h)}{\tfrac{1}{2}(h)^2(h_{k-1}+h)^2}\right]}^{\eta}$$

$$-\overline{\left[\sum_{k=1}^{K-1}[\sigma_{k-1}-\sigma_{k}](\nu_u)'\frac{\overline{\nu_v}^{\xi}(u'-u'_{k+1})(2h+h_{k+1})}{\tfrac{1}{2}(h)^2(h+h_{k+1})^2}\right]}^{\eta}$$

$$-\overline{\left[\sum_{k=1}^{K-1}[\sigma_{k}-\sigma_{k+1}](\nu_u)'\frac{\overline{\nu_v}^{\xi}(u'-u'_{k+1})}{\tfrac{1}{2}h(h+h_{k+1})^2}\right]}^{\eta}$$

$$+\overline{\left[\sum_{k=2}^{K}[\sigma_{k-2}-\sigma_{k-1}](\nu_v)'\frac{\overline{\nu_v}^{\eta}(v'_{k-1}-v')}{\tfrac{1}{2}h^{v}(h^{v}_{k-1}+h^{v})^2}\right]}^{\xi}$$

$$+\overline{\left[\sum_{k=2}^{K}[\sigma_{k-1}-\sigma_{k}](\nu_v)'\frac{\overline{\nu_v}^{\eta}(v'_{k-1}-v')(h^{v}_{k-1}+2h^{v})}{\tfrac{1}{2}(h^{v})^2(h^{v}_{k-1}+h^{v})^2}\right]}^{\xi}$$

$$-\overline{\left[\sum_{k=1}^{K-1}[\sigma_{k-1}-\sigma_{k}](\nu_v)'\frac{\overline{\nu_v}^{\eta}(v'-v'_{k+1})(2h^{v}+h^{v}_{k+1})}{\tfrac{1}{2}(h^{v})^2(h^{v}+h^{v}_{k+1})^2}\right]}^{\xi}$$

$$-\overline{\left[\sum_{k=1}^{K-1}[\sigma_{k}-\sigma_{k+1}](\nu_v)'\frac{\overline{\nu_v}^{\eta}(v'-v'_{k+1})}{\tfrac{1}{2}h^{v}(h^{v}+h^{v}_{k+1})^2}\right]}^{\xi}$$

$$-\overline{\left[[\sigma_{K-1}-\sigma_{K}](\nu_u)'_{K}\frac{g}{C^2}\frac{u'_{K}\sqrt{(u_K)^2+(\overline{v'_K}^{\eta\xi})^2}}{(h_K)^2}\right]}^{\eta}$$

$$-\overline{\left[[\sigma_{K-1}-\sigma_{K}](\nu_v)'_{K}\frac{g}{C^2}\frac{v'_{K}\sqrt{(v_K)^2+(\overline{u_K}^{\xi\eta})^2}}{(h^{v}_K)^2}\right]}^{\xi}$$

4.4.3. Vertical viscosity

The differential of an additive control parameter (which is time-independent) defined for eddy viscosity in the first stage is given by:

$$-\overline{\left[\sum_{k=2}^{K}\frac{(\nu_u)''(u''_{k-1}-u'')}{\frac{1}{2}h'(h'_{k-1}+h')^2}\right]^{\xi}}+\overline{\left[\sum_{k=1}^{K-1}\frac{(\nu_u)''(u''-u''_{k+1})}{\frac{1}{2}(h')^2(h'+h'_{k+1})^2}\right]^{\xi}}$$

$$-\overline{\left[\sum_{k=2}^{K}\frac{(\nu_v)''(v''_{k-1}-v'')}{\frac{1}{2}h'^{,v}(h'^{,v}_{k-1}+h'^{,v})^2}\right]^{\eta}}+\overline{\left[\sum_{k=1}^{K-1}\frac{(\nu_v)''(v''-v''_{k+1})}{\frac{1}{2}(h'^{,v})^2(h'^{,v}+h'^{,v}_{k+1})^2}\right]^{\eta}}$$

The differential of an additive control parameter (which is time-independent) defined for eddy viscosity in the second stage is described by:

$$-\overline{\left[\sum_{k=2}^{K}\frac{(\nu_u)'(u'_{k-1}-u')}{\frac{1}{2}h(h_{k-1}+h)^2}\right]^{\xi}}+\overline{\left[\sum_{k=1}^{K-1}\frac{(\nu_u)'(u'-u'_{k+1})}{\frac{1}{2}(h)^2(h+h_{k+1})^2}\right]^{\xi}}$$

$$-\overline{\left[\sum_{k=2}^{K}\frac{(\nu_v)'(v'_{k-1}-v')}{\frac{1}{2}h^v(h^v_{k-1}+h^v)^2}\right]^{\eta}}+\overline{\left[\sum_{k=1}^{K-1}\frac{(\nu_v)'(v'-v'_{k+1})}{\frac{1}{2}(h^v)^2(h^v+h^v_{k+1})^2}\right]^{\eta}}$$

4.5. Remarks on WAQAD with respect to TRIWAQ

The remarks on WAQAD with respect to TRIWAQ are:

- The 3D WAQAD bottom friction terms fruu3D, fruv3D, frvu3D and frvv3D described at the end of section 4.3 contain a shift of half a time level with respect to the bottom friction terms in TRIWAQ. In the term frwl3D the shift of half a timelevel with respect to TRIWAQ is corrected.

- Horizontal and vertical advection is not included in WAQAD, but it is in TRIWAQ.

- Horizontal viscosity is not included in WAQAD, but it is in TRIWAQ.

- Just as in the case of WAQUA, additional features of TRIWAQ are not included in WAQAD. This may lead to the same problems described in section 3.5. The features of concern are:
  - External forcings like wind, discharges and density gradient.
  - Transports, STRESS2d, barriers and weirs.
  - Smoothing boundary values.
  - Depth multiplier.

- In TRIWAQ there are two ways to prescribe layers: fixed layers or sigma layers. WAQAD assumes that no fixed layers are prescribed in the forward model.

- Just as WAQUA, TRIWAQ writes map data only at every whole time step and not every half time step. In WAQAD the map data at whole time steps is interpolated to half time steps.

5. Possibilities, options and shortcomings

In this chapter the possibilities, options and shortcomings of WAQAD regarding the following subjects are discussed:

- Identifiability and the use of the penalty (section 5.1)
- The use of weighting functions for parametrization (section 5.2)
- Coupling harmonic constituents (section 5.3)
- Analysis of the gradient in time and space (section 5.4)
- The use of current-velocity measurements (section 5.5)
- Friction formulations (section 5.6)
- Finite difference calculations (section 5.7)
- Velocity and discharge boundaries (section 5.8)

5.1. Identifiability and the use of the penalty

5.1.1. Introduction

When a model is calibrated automatically it is possible for several combinations of parameters to result in the same (minimal) value of the cost function. This is called an identifiability problem (I-problem). In such cases it is impossible to find the 'right' values of the parameters, because there are not enough observations (or the observations are not appropriate) to estimate the parameters. In general one can indicate locations at which observations could be obtained to solve the I-problem. However, it is not practical to try to solve every I-problem with extra data.

Instead of solving the I-problem, the input - that is the description of the parameters to be estimated - can be changed. For example it is impossible to estimate the bottom depth using only a few measurement stations, bu it is possible to estimate the average bottom depth instead. Reducing the number of parameters will generally lead to a better estimation problem. And using a method called the penalty can also solve some I-problems.

5.1.2. Some examples

The following examples using a simple linear one-dimensional problem illustrate a number of I-problems that can occur during the WAQAD calibration process. Figure 5.1 shows a one-dimensional problem with an open boundary on the left-hand side and a solution that converges to zero at infinity (on the right-hand side). This problem illustrates, for example, a Kelvin wave that progresses counter clockwise through the North Sea, with the x-axis following the coast line.

The equations are described by a simple linear version of the shallow water flow equations:

$$\frac{\partial \zeta}{\partial t} + D\frac{\partial u}{\partial x} = 0$$

$$\frac{\partial u}{\partial t} + g\frac{\partial \zeta}{\partial x} + \frac{f}{Du} = 0$$

$$\zeta(0,t) = H_0 \sin(\omega t - \phi_0)$$

$$\lim_{x\to\infty} \zeta(x,t) = 0 \qquad (5.1)$$

The solution to this problem (at constant depth) in first order is given by:

$$\zeta(x,t) = H_0 \sin\left(\omega(t - \frac{x}{\sqrt{Dg}}) - \phi_0\right) e^{-\left(\frac{f\sqrt{g}}{2\sqrt{D}}\right)x} \qquad (5.2)$$

with a linear friction with coefficient f (f is small).

In this solution a harmonic wave is recognized which progresses from the left to the right at velocity $\sqrt{gD}$ en which is slightly attenuated.

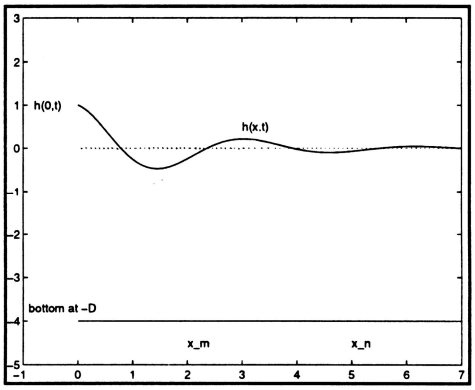


figure 5.1 A simple problem

I-problem 1: phase at the boundary and depth

Suppose there is only one water level station in $x=x_m$. At this station a sinusoidal signal obscured by noise is measured. Equation (5.2) shows that the phase of this signal is determined solely by the phase at the boundary and the transit velocity of the wave, that is the depth. The amplitude of this signal is also dependent on the depth but not on the phase at the boundary. This means that in principle the depth can be estimated in this way when the friction is known. If the friction is unknown or not accurately known then every combination of the depth and the phase at the boundary that leads to the correct phase at the measurement point will minimize the cost function. This means that there is an I-problem. Figure 5.2 shows the progress of the cost function schematically. In general an I-problem can be recognized from a graph if it shows a long drawn-out decline with at least one direction in which the cost hardly varies. Unfortunately, in practice it is not possible to produce such a picture for several reasons. For example, evalution of the cost function at one point requires much computational time. Performing the dozen evaluations necessary in the case of two dimensional

pictures, is already stretching the limit of computational possibilities. And the number of evalutions required increases explosively when the number of parameters increases.

Because of the measurement noise the cost function will differ slightly from its theoretical minimum value (see figure 5.3). It is obvious that even a small measurement noise will lead to a large variation in the minimum point in the case of an I-problem. The solution (estimation) will vary, especially in the direction of the descent, since a slight vertical change will have a large effect on the minimum because of the measurement noise. This increases the noise in this direction.

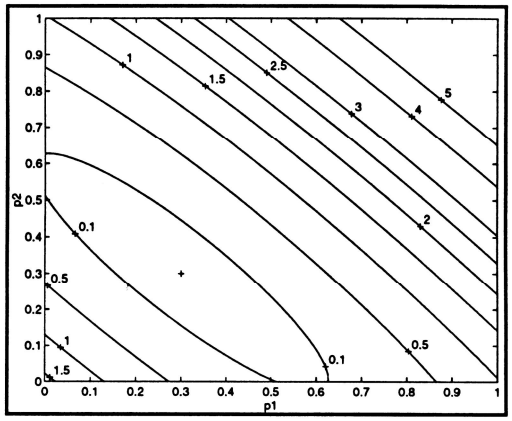


figure 5.2 An example of a cost function for an I-problem

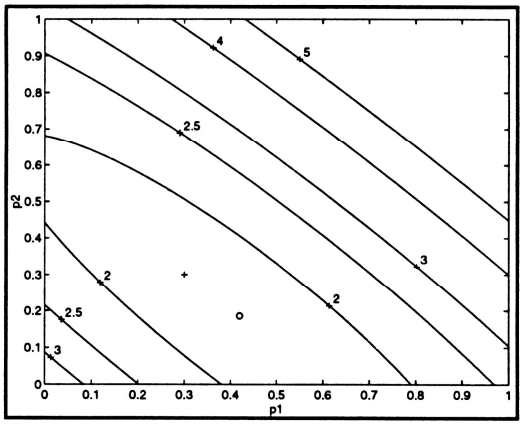


figure 5.3 Change in the cost function for an I-problem due to noise

I-problem 2: two depth boxes between two measurement stations

Consider the situation of I-problem 1. In this case there is a second water level station at $x=x_n$. We assume that $x_m \approx 0$ (measurements are made at the boundary) which means that the phase at the boundary is supposed to be known. The depth is divided into two boxes: one box from x_m to $x_{between}$ (no measurements are made at $x_{between}$) and one box from $x_{between}$ to x_n ($x_m<x_{between}<x_n$). The phase of the signal at x_n is now determined by the phase at the boundary (known to a greater or lesser extent) and the transit time from the boundary to x_n. The transit time is the sum of the transit times in the two boxes. The phase in x_n is thus:

$$\phi_n = \phi_0 + \frac{\omega(x_{between} - x_m)}{\sqrt{D_1 g}} + \frac{\omega(x_n - x_{between})}{\sqrt{D_2 g}} \qquad (5.3)$$

The separate transit times and with them the depths are not to be estimated. Each combination of depths with the same total transit time has the same value of the cost function, which means that there is an I-problem. If the phase at the boundary does not have to be estimated, it is not necessary for x_m to be at the boundary. This means that this problem can also occur at another place in the model.

I-problem 3: harmonic constituents that are difficult to separate

It is a known fact that harmonic constituents with frequencies which are close together can only be separated using long series of measurements. This is still a problem when WAQAD is used. It is regarded here as an I-problem. See section 5.3 for more information on solving this problem.

I-problem 4: more boundary points than stations

It is possible to prove that estimation of the constituents at the boundary leads to an I-problem if there are more boundary points than measurement points. However, the proof is very technical (mathematically) and has therefore been omitted.

5.1.3. Splitting the calculation

The number of parameters to be estimated is sometimes so very large that is is tempting to break down the calibration process into a number of steps. The resulting separate problems are smaller and therefore require less computational time. For example, one could first calibrate the constituents of the open boundary and next the bottom depth and friction. Note, however, that such a procedure could conceal the I-problem.

For example, look at the cost function in figure 5.2 and consider the problem of calibrating parameter p_1 only. Figure 5.4 shows the corresponding cost function with a clear minimum. Minimizing of the second parameter (figure 5.5) using the minimum for the first parameter results in a clear minimum again and the whole I-problem seems to have disappeared. However, this is not so: the problem is still there. The advantage is that the observation errors are less amplified, resulting in adaptations which will not be unrealistically large. However, it is not possible to recognize an I-problem right away unless the calibration process is iterative (after calibrating parameter p_2 parameter p_1 is calibrated again and so on). Figure 5.6 shows the progress of the iterative procedure.

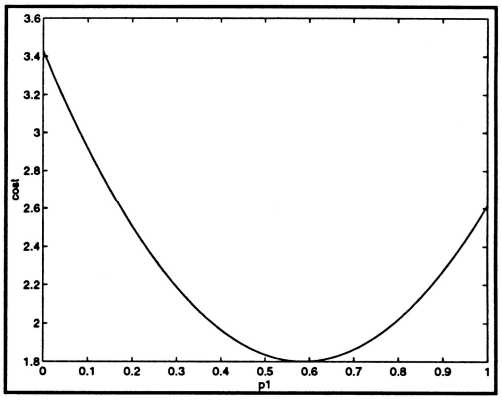


figure 5.4 Cost for parameter 1 only

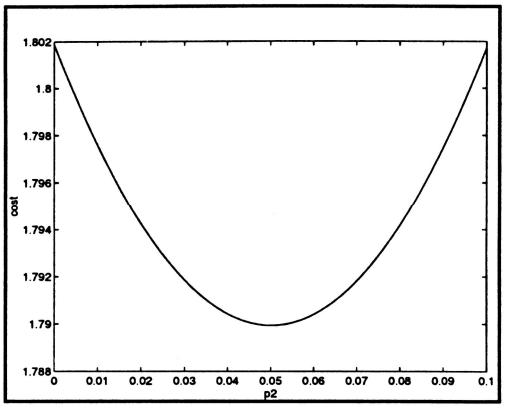


figure 5.5 Cost for parameter 2 only

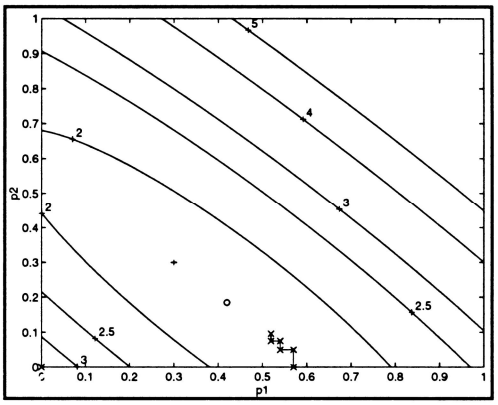


figure 5.6 Progress of the iterative procedure

5.1.4. Validation of the calculation process

Since it is impossible to determine beforehand if an I-problem will occur, it would be practical to ascertain if all is still going well during the optimization process (the execution of the calculation). Two methods seem feasible at this moment:

Using two data sets

If two data sets are available, one can be used for calibration. The cost function of the other set could be reproduced in a graph in order to check the first set. The second data set can also be obtained by splitting one data set (in time or into stations). Figure 5.7 shows an example of both graphs.

Using the steepest descent method (for BFGS too), the steepest direction of the descent will be followed in the first iteration. In these directions (iterations) the model will really improve and the cost function of the control data will also decrease. After a number of iterations no steepest directions remain and then the direction of the line of the descent will also be searched. In this direction the cost function will decrease slightly, but the improvement is only cosmetic because of the observation errors. In fact, the model will get worse and the cost function of the control data will increase.

Using estimation of the Hessian

The convexity of the cost function at its minimum can be searched by means of the second order derivative of the cost function (Hessian). The contour lines of the cost function in the neighbourhood of the minimum are approximately elliptical. The directions of the axes of these ellipses are formed by the eigenvectors of the inverse of the Hessian and the ratios of the lengths of the axes are formed by the ratios

of the square roots of the eigenvalues of the inverse of the Hessian. Figure 5.8 shows the eigenvectors scaled by the square roots of the eigenvalues.

It is clear that the occurrence of an I-problem can be characterized by the presence of large eigenvalues of the inverse. In practice 'large' is probably best described relative to the other eigenvalues.

During the iteration process of the BFGS algorithm an increasing part of the inverse of the Hessian is estimated. The occurrence of large eigenvalues in this estimation seem a reasonable indication of the occurrence of an I-problem.

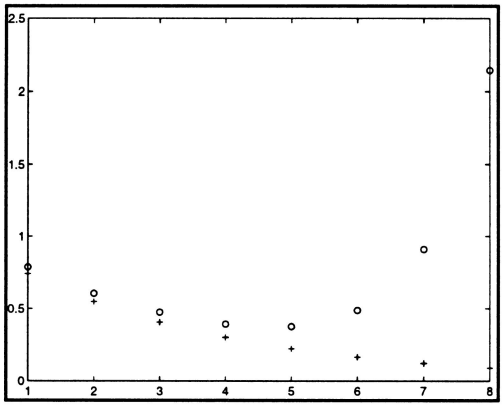


figure 5.7 Cost function for measurements to be calibrated (+) and control measurements (o)

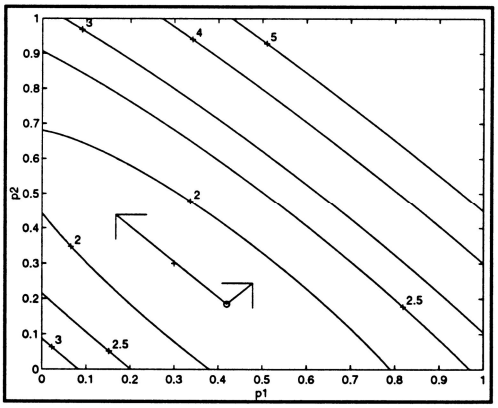


figure 5.8 Eigenvectors and eigenvalues

For more information on the use of the Hessian, see subsection 5.4.6.

5.1.5. Regularization

Methods for giving the cost function a more regular progress without causing I-problems are often called regularization methods. One such method will be described briefly in this subsection. The other method, called the penalty, will be described in detail in the next subsection.

Reduction of the number of parameters

If an I-problem is caused by choosing too many parameter boxes for depth or friction, it can be solved by reducing the number of boxes, for example by fusing them. Suppose that the calculation from I-problem 2 has a cost function shown by figure 5.2. Fusing the two boxes results in both parameters being adapted by the same value. In this way, only the line $p_1=p_2$ is searched. Figure 5.9 shows the resulting cost function. The I-problem is solved in this way. The problem is solved in a mathematical sense, but it is of course extremely important that the constant adaptation over the large (fused) box is a reasonable assumption.

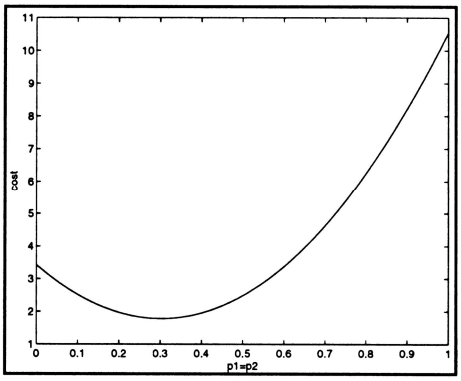


figure 5.9 Cost function for the joined parameters

5.1.6. Penalty for deviation from prior estimates

5.1.6.1. Introduction

In some cases the standard quadratic cost does not lead to acceptable results. In such cases the adaptations of some parameters are unreasonably large while others are quite acceptable. This is not a feature of the algorithms used but it is inherent to the problem.

The adaptations of the parameters are based solely on the values of the waterlevels measured at certain points in the model. Sometimes it is attempted to adapt a parameter that

cannot be estimated well from the data. For example, it is clearly not possible to estimate the depth of the bottom near Denmark from data on the English and Dutch coasts, since changing the depth at the Danish coast has hardly any influence on water levels at the Dutch coast. Data obtained near the area in question are needed to solve this problem. Alternatively, the estimation of the depth near Denmark can be omitted. This will make the other estimations behave better.

The situation becomes more complicated if a combination of parameters cannot be estimated. For example, trying to estimate depth, friction and the phase of the boundary conditions simultaneously from data from only waterlevelstation, can lead to the following problem. If the tidal wave arrives too early at the measurement station this can be due to the wave velocity or to the phase at the boundary. Now the adaptation routine does not know which of the two parameters to adapt. In an attempt to solve this problem the method will change both slightly. This part is inherent to the problem and more data is needed to solve it.

The biggest problem, however, is that it is possible to adapt the depth and the phase at the boundary such that the model predictions at the measurement point do not change. This kind of problem can give very large and unrealistic values for the parameters.

Various ways of dealing with these problems have been suggested in the literature, [Verlaan, 1994] and [Verlaan, 1996]. Most can be written as the addition of an extra term to the cost function. This additional term will be called penalty from now on. This penalty often takes one of two forms. One way is to penalize large adaptations, for example by adding a penalty that is proportional to the square of the change in the parameters. The second is meant for parameters that describe the spatial distribution of a certain property (like depth). Here, usually differences between adaptations that are close in space receive a penalty. The result of this last type is a more regular distribution of the parameters in space. A combination of these two types of penalties usually creates a better conditioned problem and solves the problem of unrealistic adaptations.

In the case of the first example, the cost hardly changes from the adaptations at the Danish coast while the penalty becomes large, which results in a large total cost (cost plus penalty). The minimum total cost will now be attained with smaller adaptations.

In the second example, large adaptations that give the same cost will now be given a large total cost and thus these adaptations will not be made by the algorithm. This shows on

one hand that there will be no unrealistic adaptations but on the other that there still is not enough data to make the correct adaptations.

The two examples above were of course unrealistic. But problems like this often occur in less obvious forms. Often - but not always - they occur when we want to estimate too many parameters with too few data.

The second motivation for using a penalty can be that this enables the user to select which parameters are known well or which parameters are known with less accuracy. Often one knows from the way in which the data are obtained which parameters in the model are known accurately and which are not. For example, depths can be measured quite well, while bottom friction measurements are difficult to obtain. This also implies that larger adaptations are acceptable for bottom friction values than for depth values. By adjusting the penalty all this information can be used.

The disadvantage of using a penalty is that one or more parameters for this penalty need to be specified. Often these settings can only be obtained by experimenting with different values and selecting a value that gives reasonable results. The method described here, however, requires parameters to be in a form that can easily be interpreted and the values can often be guessed instantly from experience or information about the accuracy of the data used.

The arguments in this introduction show that the penalty can be useful for solving a number of problems. However not all problems are solved automatically. Some can only be solved by using more data (or data at better chosen points in space or at better times).

5.1.6.2. Theoretical background

The cost criterion used in WAQAD is quadratic and can be viewed as a Maximum Likelihood estimator. In this framework the addition of a penalty is simply the transition from a Maximum Likelihood esitmator to a Bayesian estimator.

The prior probability distribution needed for the Bayesian estimator can, under the assumption that it is Gaussian, be characterized by its mean and covariance. This covariance is computed with a model to assist the user in building this matrix.

More precisely: If p is the parameter vector and y(t,p) are the model results computed with these parameters at time t, and $y_o(t)$ are the measured values, then the quadratic cost criterion was:

$$J(p) = 0.5 \sum_{t \in T} (y(t,p) - y_o(t))^2 \tag{5.4}$$

On the other hand if we assume that the measurement errors of $y_o(t)$ are Gaussian and identically distributed with mean 0 and standard deviation σ the Maximum Likelihood estimator can be written as:

$$L(p) = \prod_{t \in T} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(y(t,p) - y_o(t))^2}{2\sigma^2}} \tag{5.5}$$

Taking minus the logarithm of this expression reduces it to the 'old' criterion for all σ.

Bayesian estimation is a logical extension of Maximum Likelihood estimation that is based on Bayes's rule, which reads:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \tag{5.6}$$

This can be seen easily from the definition of conditional probability:

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \tag{5.7}$$

if we apply this to our estimation problem we get:

$$P(p = p^* \mid y(t,p) = y_o(t);\ t \in T) = \frac{\prod_{t \in T} P(y(t,p) = y_o(t)) P(p = p^*)}{\int \prod_{t \in T} P(y(t,p) = y_o(t)) P(p = p^*) dp} \tag{5.8}$$

if for the prior distribution P(p=p*) we assume that it is Gaussian distributed with mean 0 and covariance C and note that the denominator does not depend on p. By also taking the minus logarithm we can obtain:

$$J(p)=\sum_{t\in T}\frac{(y(t,p)-y_o(t))^2}{\sigma^2}+p'C^{-1}p \qquad (5.9)$$

This looks very much like the Maximum Likelihood estimator. The only difference is the penalty $p'C^{-1}p$. It can be shown that this penalty is always positive. So instead of minimizing the cost we now try to minimize the total cost, which means cost plus penalty.

If the prior is taken uniform over p (independent of p) the Bayesian estimator reduces to the Maximum Likelihood estimator. This can be interpreted as there being no prior information on parameters or, all parameters are equally probable before the results of the simulation are known.

The routines for using penalty functions also provide some help in generating the covariance matrix C. The model used for parameters that in principle could vary for all x and y coordinates is based on the spatial distribution of the parameters. These parameters (for example, the values for depth and bottom friction) are parametrized using rectangles or triangles. But this is just for the program. For the original data we can characterize the error structure by the variance of the parameters at a point and the correlation between two points. This correlation (to what extent the points depend on each other) decreases with increasing distance between the points. Thus if we measure the depth somewhere near Scheveningen with an error of one metre (too deep) we cannot say anything about the error of a measurement obtained somewhere near Bergen (Norway), but a depth measurement obtained near Hoek van Holland will probably be to deep too. The range within which two measurements influence each other is called the characteristic distance of the error.

Let Q be a parameter that depends on the spatial variables x and y, that take only discrete values. Assuming that all these stochastic variables are jointly Gaussian with expectation 0 then the probability density is fully described by the variances of Q(x,y), the correlations between any two points and the zero mean. We model the correlation of the error in Q, denoted by ΔQ, between the points (x_1,y_1) and (x_2,y_2) as:

$$\mathrm{corr}(\Delta Q(x_1,y_1),\Delta Q(x_2,y_2))=e^{-\frac{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2}}{d}} \qquad (5.10)$$

The parameter d serves as a characteristic distance (see figure 5.10). This distance indicates over what order of length the correlation is significant. The method used for measurements (for example, of depths) may indicate reasonable values for this. In our experience one tenth of the model diameter is a good default when no accurate information is available. When other coordinates are used the distance in the numerator of the exponent of equation (5.5) may be defined differently.

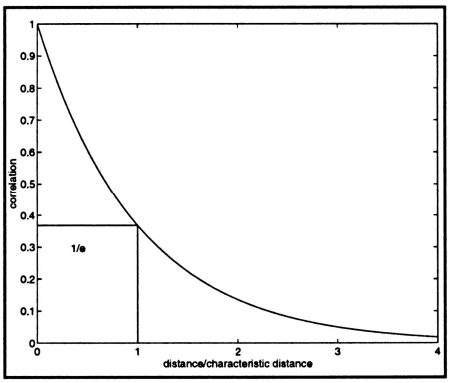


figure 5.10 Correlation and characteristic distance

The correlation in the a priori errors is important for two reasons. The errors are not considered to cancel each other out when averaged over an area and the resulting penalty is large when two points close together are adapted in different directions.

The parameters λ_i that are used by the program can be characterized by a set of weighting functions (5.2) $g_i(x,y)$. The adaptations made to the model can always be written as a linear combination of these functions:

$$\Delta Q\,(x, y) = \sum \lambda_i\, g_i\,(x, y) \qquad (5.11)$$

If the g_i form a linear set of basic functions over all x,y then there is a linear one to one correspondence between λ_i and the ΔQ. We can rewrite the above operation as a matrix multiplication with ΔQ denoting a vector that stores all $\Delta Q(x,y)$ and λ containing all λ_i:

$$\Delta Q = G\,\lambda \qquad (5.12)$$

The covariance of the λ_i can now be calculated by:

$$E\,[\lambda\lambda'] = G^{-1} E\,[\Delta Q \Delta Q'](G^{-1})' \qquad (5.13)$$

Since we usually only want to use a few functions g_i we do not have a linear basis and thus we cannot invert G. But we can estimate λ from ΔQ using the least squares method:

$$\lambda = (G'G)^{-1}G'\Delta Q \tag{5.14}$$

Using this formula we estimate the variance of λ from the variance in ΔQ:

$$E[\lambda\lambda'] = (G'G)^{-1}G'E[\Delta Q\Delta Q']G(G'G)^{-1} \tag{5.15}$$

This is the method used in the program to compute the covariance matrix needed for the penalty. The symmetry of covariance matrices can be exploited to reduce the time needed for computation. The algorithm becomes slightly more complicated due to the indirect storage of the WAQUA-in-SIMONA and WAQAD programs.

The indirect specification of the covariance matrix for the penalty has some important advantages over a direct specification. The parameters that have to be given by the user have a clear interpretation and the penalty is independent of the parameterization. The latter means that when for instance a rectangle is divided into two smaller rectangles and the adaptations of the two rectangles are equal the penalty equals the penalty of the original situation. In this case also, any difference between the adaptation of the two rectangles receives an additional penalty.

5.1.6.3. Practical use

Although it is very important to understand the mathematics of the penalty in order to derive the formulas, to use the penalty it is sufficient to understand what it does rather than how it does it. In general the penalty will not allow adaptations that are too large. What is considered too large can be controlled by the standard deviations and characteristic lengths that are required in the input. Usually it will suffice to take reasonable values known from experience or intuition. The result of the adaptation process should mostly not be very sensitive to the exact values.

However, if the adaptations after a first run are too large or too small for the user, this can be changed. How the input of WAQAD affects the adaptations is explained in detail in the WAQAD User's Guide and [Verlaan, 1994]. In [Verlaan, 1996] the use of the penalty is also illustrated by means of an experiment.

5.1.7. Conclusion

The WAQAD program always gives output to the input of a calibration problem. Also the calculated solution is always better if a comparison is made using the measurements that are assimilated by WAQAD. However, the calibrated model is not always really better. It is therefore very important to be able to analyse in which cases WAQAD can be used in a useful way or how the problem can be changed in such a way that WAQAD is useful.

Using a penalty enables a number of problems to be avoided. Large unrealistic adaptations are no longer possible and, furthermore, large differences in adaptations for points that are close to each other will be prevented. The penalty gives us the freedom to indicate which parameters are known accurately or not. If desired, this can be used to stress certain aspects of the model. Although in many cases the results will now be acceptable to the user it remains important to have many well spread data available. Only parameters that affect the results of the simulation at the points and times of the measurements can be estimated.

5.2. The use of weighting functions for parametrization

5.2.1. Introduction

When trying to identify a parameter (here denoted by Q) that depends on spatial coordinates, a set of weighting functions needs to be selected to specify the types of adaptations that are allowed for changing the initial estimate. The adaptation becomes a linear combination of the weighting functions $g_i(x,y)$:

$$\Delta Q(x, y) = \sum \lambda_i g_i (x, y) \qquad (5.16)$$

This equation can also be written in matrix notation:

$$\Delta Q = G \Lambda \qquad (5.17)$$

Where Q is a column vector that contains the Q(x,y), the columns of G contain the weighting functions and Λ is a column vector with all the parameters.

Several types of weighting functions have been suggested in the literature such as: point functions, rectangles, triangles, splines and other functions fitted to the problem. A description of all the weighting functions mentioned is given in [Verlaan, 1994]. Rectangles and triangles are implemented in the WAQAD system. These weighting functions are described below:

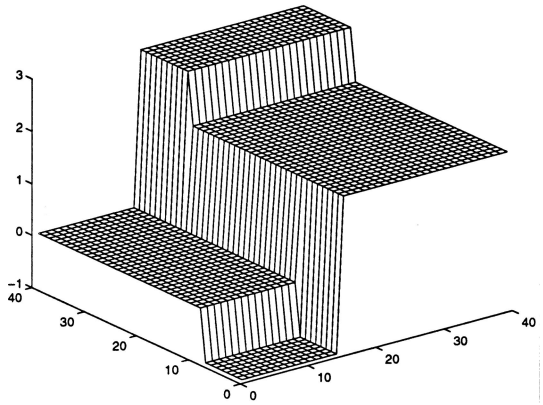


figure 5.11 Rectangles

- Rectangles. Every weighting function is one of a set that is composed of rectangles and is zero outside this set. These are the weighting functions that were initially used in the WAQAD system. Their great advantage is that they are easy to compute and many algorithms that use the weighting functions can take advantage of the special structure. Their disadvantage is that at certain edges the

adaptations jump from one value to another. These discontinuities may cause problems, since waves are partially reflected at these edges. These reflections are an artefact of the model. They do not exist in reality. The discontinuities are also very different from the physical situation, where there are no jumps along straight lines.

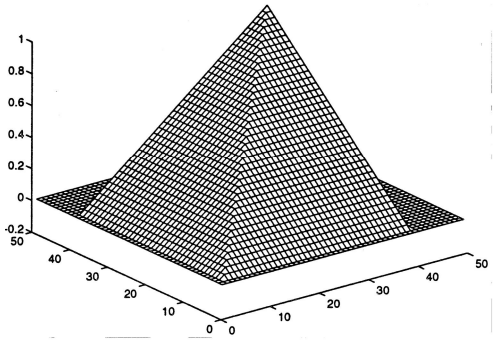


figure 5.12 Triangles

- Triangles, where the weighting functions are pyramids. The resulting adaptation is a linear interpolation of the values on the edges of a set of triangles in space. This type of representation is well known for its use in finite element methods for partial differential equations. With some caution, the adaptations at the boundary are always continuous. An additional advantage is that the geometry can be followed more easily using triangles than using rectangles.

In the next part of this section the extension of the WAQAD system for triangles is described. Triangles have been chosen because the geometry is easy to follow and the algorithms are relatively simple.

5.2.2. Theoretical background in the case of triangles

Linear interpolation between the three sides of a triangle is not difficult when baricentric coordinates are used. If the three sides of a triangle are given by the Cartesian coordinates $(x_1,y_1),(x_2,y_2)$ and (x_3,y_3), then the baricentric coordinates for this triangle are given by the equations:

$$\begin{aligned} \lambda_1 x_1 + \lambda_2 x_2 + \lambda_3 x_3 &= x \\ \lambda_1 y_1 + \lambda_2 y_2 + \lambda_3 y_3 &= y \\ \lambda_1 + \lambda_2 + \lambda_3 &= 1 \end{aligned} \qquad (5.18)$$

where $(\lambda_1,\lambda_2,\lambda_3)$ are the baricentric coordinates. In baricentric coordinates linear interpolation can be written as:

$$Q(x, y) = \lambda_1 Q(x_1, y_1) + \lambda_2 Q(x_2, y_2) + \lambda_3 Q(x_3, y_3) \qquad (5.19)$$

Using the set of linear equations (5.18) and formula (5.19) Q can be evaluated at a certain point; these evaluations can then be used to construct the weighting functions. When the appropriate routines are rewritten in terms of weighting functions the transfer to triangles is straightforward, and is achieved by changing the weighting functions.

5.2.3. Computation of the gradient in the case of triangles

When a different set of weighting functions is used then the computation of the gradient needs to be changed. Let Q(x,y) be a parameter that depends on spatial coordinates (x,y) and $g_i(x,y);i=1,...,m$ a set of weighting functions for the adaptations in the parameters. The relation between the adaptation of Q(x,y) and the coefficients λ_i of the weighting functions $g_i(x,y)$ is given by:

$$\Delta Q(x, y) = \sum_{i=1}^{m} \lambda_1 \; g_1 \; (x, y) \qquad (5.20)$$

If the gradient of the criterion with respect to Q(x,y) is known then the gradient with respect to the coefficients of the weighting functions can be computed by:

$$\frac{\partial J}{\partial \lambda_i} = \sum_{x,y} g_i (x, y) \frac{\partial J}{\partial Q(x, y)} \qquad (5.21)$$

So in contrast to the use of rectangles, the summation of the gradient $\partial J / \partial Q(x, y)$, which was over the rectangle is now over the whole computational grid and there is an additional weighting function. However, in both cases the computation can be done using weighting functions.

5.2.4. Implementation in the case of triangles

For the computation of the weighting functions it is important to identify triangles with common sides are identified. Therefore the storage of the triangles is indirect. First the coordinates of the points that are sides are given together with a unique number. The triangles are now described by enumerating the numbers of the sides.

To ensure continuity on the boundaries of the region where adaptations are made, it is possible to make sides of triangles inactive as a parameter. This option can also be used to deactivate other sides when needed for some reason.

The implementation of triangles in WAQAD is described in more detail in [Rozendaal, 1995].

5.2.5. Conclusion

The use of other basic functions can improve the performance of the WAQAD system by dealing with the problem of discontinuities that are introduced when using indicator functions on rectangles as weighting functions. These new weighting functions also make it easier to follow the model geometry. When fully implemented it will probably be an improvement to the WAQAD system. It will be necessary to evaluate the performance on a real-life model, since it cannot be guaranteed that these new weighting functions will not introduce unwanted effects.

At present, rectangles and triangles are implemented in WAQAD. For a detailed description of the input requirements for these weighting functions, see the WAQAD User's Guide.

5.3. Coupling harmonic constituents

5.3.1. Introduction

The boundary conditions for many model schematizations are described by harmonic constituents. During the calibration process these boundary conditions are usually modified. The calibration can be done by hand or by using WAQAD.

The angular velocities of certain constituents are very similar, for example:

S2 = 30.00°/hour

K2 = 30.08°/hour

A minimum simulation of 360°/(30.08 - 30.00)° hours = 4500 hours ≈ half a year is required to separate these constituents. Using WAQUA models a simulation period of approximately one month is a practical limit for the computational effort. If the simulation period is too short, another way must be found to determine the amplitude ratio and the phase difference between constituents S2 and K2. One possible (partial) solution to this problem is to couple the two constituents and then consider them as a single constituent. The HATYAN program is available for coupling constituents when calibration is done by hand. This section discusses how constituents can be coupled by using WAQAD for automatic calibration.

5.3.2. Theoretical background

In this subsection the coupling of two constituents is described. However, the results described still hold if more than two constituents are coupled.

Assumptions:

Let ζ_1 en ζ_2 be two constituents in time, as follows:

$$\zeta_1(t) = A_1 \sin(\omega_1 t - \phi_1)$$

$$\zeta_2(t) = A_2 \sin(\omega_2 t - \phi_2)$$

in which:

$A_{1,2}$	amplitude $\zeta_{1,2}$
$\omega_{1,2}$	angular velocity $\zeta_{1,2}$
$\phi_{1,2}$	phase $\zeta_{1,2}$

Since the angular velocities of both constituents are not identical, the phase difference of both constituents can vary during the simulation. The longer the simulation period lasts, the bigger the variation can become. In this section it is assumed that, if the variation of the phase difference becomes more than 45^o, the constituents are too far apart to be separated. Let S be the simulation period. The next simple test must then hold:

$$(\omega_1 - \omega_2)\, S < \tfrac{1}{8}\pi \qquad (5.22)$$

Such a test does not have to be implemented for the amplitude ratio between the two constituents, for this will stay the same during the period that is considered (the amplitude is not a function of S).

Coupling the constituents:

WAQAD calculates the gradient. For the coupled constituents the gradient can be determined in two ways:

1. By deriving the gradient for the coupled constituents all over again
2. By using the gradients already derived in a considered way

The very laborious first method is not applied, since using existing knowledge an elegant derivation of the gradient can be found.

Gradient of the phase:

If $\omega_1 \approx \omega_2$, and constituents ζ_1 and ζ_2 are coupled together, the phase can be calibrated in two ways:

1. both constituents are shifted over the same phase $\Delta\phi$, that is:

$$\zeta_1(t\ ) = A_1 \sin(\omega_1 t - \phi_1 - \Delta\phi)$$

$$\zeta_2(t\ ) = A_2 \sin(\omega_2 t - \phi_2 - \Delta\phi)$$

2. both constituents are shifted over the same period T, that is:

$$\zeta_1(t\ ) = A_1 \sin(\omega_1(t - T\ ) - \phi_1)$$

$$\zeta_2(t\ ) = A_2 \sin(\omega_2(t - T\ ) - \phi_2)$$

The second method is chosen for WAQAD, for in this way the calculated signal will stay the same with respect to its shape. The gradients of the phase are then calculated by:

$$\frac{\partial J}{\partial \phi_1} = \sum_i \frac{\partial J}{\partial \zeta(t_i)} \frac{\partial \zeta(t_i)}{\partial \phi_1}$$

$$= \sum_i \frac{\partial J}{\partial \zeta(t_i)} \left(- A_1 \cos(\omega_1(t_i - T\ ) - \phi_1)\right)$$

$$\frac{\partial J}{\partial \phi_2} = \sum_i \frac{\partial j}{\partial \zeta(t_i)} \left(- A_2 \cos(\omega_2(t_i - T\ ) - \phi_2)\right)$$

and the gradient to T:

$$\frac{\partial J}{\partial T} = \sum_i \frac{\partial J}{\partial \zeta(t_i)} \left(\frac{\partial \zeta_1(t_i)}{\partial T} + \frac{\partial \zeta_2(t_i)}{\partial T} \right)$$

$$= \sum_i \frac{\partial J}{\partial \zeta(t_i)} \left(\frac{\partial}{\partial T}(A_1 \sin(\omega_1(t_i - T\ ) - \phi_1) + \frac{\partial}{\partial T}(A_2 \sin(\omega_2(t_i - T\ ) - \phi_2) \right)$$

$$= \sum_i \frac{\partial J}{\partial \zeta(t_i)} \left(- A_1 \omega_1 \cos(\omega_1(t_i - T\ ) - \phi_1) - A_2 \omega_2 \cos(\omega_2(t_i - T\ ) - \phi_2)\right)$$

From this it follows that:

$$\frac{\partial J}{\partial T} = \omega_1 \frac{\partial J}{\partial \phi_1} + \omega_2 \frac{\partial J}{\partial \phi_2}$$

Both constituents can thus be summarized with weights ω_1 en ω_2 (for ζ_1 and ζ_2 respectively).

The adaptations of the phases are applied to $\Delta\phi_1$ and $\Delta\phi_2$ in the following way:

$$\Delta\Phi_1 = \omega_1 \Delta T \quad \text{and} \quad \Delta\Phi_2 = \omega_2 \Delta T$$

It is useful (and numerically desirable) to normalize T with:

$$\omega \approx \omega_1 \approx \omega_2 \quad \text{such that} \quad \phi = \omega T$$

ω is described by the mean of ω_1 and ω_2, which gives:

$$\frac{\partial J}{\partial \phi} = \left(\frac{\omega_1}{\omega}\right) \frac{\partial J}{\partial \phi_1} + \left(\frac{\omega_2}{\omega}\right) \frac{\partial J}{\partial \phi_2}$$

the weights are therefore $\left(\frac{\omega_1}{\omega}\right)$ and $\left(\frac{\omega_2}{\omega}\right)$ (they will be approximately 1).

The adaptations in this case are:

$$\Delta\phi_1 = \left(\frac{\omega_1}{\omega}\right) \Delta\phi$$

$$\Delta\phi_2 = \left(\frac{\omega_2}{\omega}\right) \Delta\phi$$

with the new parameter $\Delta\phi$.

Gradient of the amplitude:

The amplitude is calibrated by calibrating variables ξ_1 and ξ_2 in the following way:

$$\zeta_1(t) = A_1 (1 - \xi_1) \sin(\omega_1 t - \phi_1)$$

$$\zeta_2(t) = A_2 (1 - \xi_2) \sin(\omega_2 t - \phi_2)$$

The gradients of the amplitude are:

$$\frac{\partial J}{\partial \xi_1} = \sum_i \frac{\partial J}{\partial \zeta(t_i)} \frac{\partial \zeta(t_i)}{\partial \xi_1}$$

$$= \sum_i \frac{\partial J}{\partial \zeta(t_i)} \left(- A_1 \sin(\omega_1 t_i - \phi_1)\right)$$

$$\frac{\partial J}{\partial \xi_2} = \sum_i \frac{\partial J}{\partial \zeta(t_i)} \left(- A_2 \sin(\omega_2 t_i - \phi_2)\right)$$

If $\omega_1 \approx \omega_2$, and constituents ζ_1 en ζ_2 are coupled, $\xi_1 = \xi_2 = \xi$ holds. The gradient to ξ is equal to:

$$\frac{\partial J}{\partial \xi} = \sum_i \frac{\partial J}{\partial \zeta(t_i)} \left(- A_1 \sin(\omega_1 t_i - \phi_1) - A_2 \sin(\omega_2 t_i - \phi_2)\right)$$

from which it follows that:

$$\frac{\partial J}{\partial \xi} = \frac{\partial J}{\partial \xi_1} + \frac{\partial J}{\partial \xi_2}$$

The gradients for the percentual adaptation of the amplitude can thus be summarized without using weights. The adaptations are:

$$\Delta \xi_1 = \Delta \xi_2 = \Delta \xi$$

5.3.3. Implementation

The constituents are coupled in WAQAD as follows:

- If the test defined by (5.22) fails for the constituents to be coupled, the preprocessor of the program gives a warning.
- Regarding the existing calculation of the gradient an extra step is implemented in order to be able to summarize some gradients by using weights.
- Just before adaptation the coupled variables (ξ and ϕ) are decoupled (to ξ_1, ξ_2, ϕ_1, ϕ_2). Then the adaptation is applied to these decoupled variables.

For more information on the implementation of coupling constituents, see [Rozendaal, 1995].

5.4. Analysis of the gradient in time and space

5.4.1. Introduction

The gradient of the criterion with respect to the parameters is an important element of the procedure for estimating parameters using a cost criterion and the adjoint model. In fact, the main purpose of the adjoint model is to compute the gradient of this criterion. This gradient gives information on the direction in which the parameters should be adapted to decrease the value of the criterion, which in turn brings about an improvement of the model. This is in fact how the gradient is used for parameter estimation.

Another interpretation of the gradient of the criterion is the local sensitivity of the quality of the model to the corresponding parameters. If a large element of the gradient is associated with a certain parameter, this indicates that a small change in this parameter has a large effect on the model. If this parameter represents an area of the depth parameter in the model, the model is sensitive to a change of the depth in that area. This enables different areas to be compared and a simple map to be made of the sensitivity over the spatial domain. One of the purposes of the programs described in this section is to provide an automatic procedure for making these maps.

As a result of the chain rule of derivatives the effect of combining two areas (parameters) into one is the weighted (using the area) average of the two elements of the gradient. If we have a map in which the areas consist of points, the gradient for an area can be found by summing the derivatives of all the points in the area. If we select an area with average derivative zero, the gradient over this area will be zero, even if the derivatives themselves are not. Clearly, this is not what we want, since the parameter appears to be optimal because the derivative is zero. But other areas can be selected that improve the model further.

The contributions to the gradient can be split in time as well as in space. The resulting function of time can be interpreted as the effect on the gradient if the parameter were changed during a short period around the time in question. For some parameters this interpretation may seem hypothetical, but the information obtained can be useful even in these cases. The programs described in this section enable graphs to be made of the gradient of parameters split as a function of time.

One direct application of the gradient split as a function of time is when selecting the period for the estimation. First notice that only the average of the function is important for the gradient itself. To obtain an accurate 'estimate' of the

gradient, the average to variance ratio should be sufficiently large. When the signal to noise ratio is large a short period is enough, but when the signal to noise ratio is small a long period is needed. Of course, this ratio is not the only aspect for the selection of the period; for instance, the characteristic times of the model are important too.

It is important to note that the gradient only gives local information. When the model is changed, eg due to WAQAD, the gradient can be very different.

The computation of the gradient split in time or space is explained below. However, it should be stressed that this procedure is largely intended as a research tool because not all implications have been worked out and neither can a clear-cut algorithm for its use be given.

5.4.2. Theoretical Background

Chain rule

The computation of the gradient split in space or time is based on the chain rule for derivatives. This rule is given by:

$$\frac{\partial f(g_1(x), \ldots, g_n(x))}{\partial x} = \sum_{i=1}^{n} \frac{\partial f(y_1, \ldots, y_n)}{\partial y_i} \frac{\partial g_i(x)}{\partial x} \qquad (5.23)$$

evaluated for $y_i = g_i(x)$.

Let Q(x,y) be a parameter that depends on the spatial variable and parameters λ_i that represent the combined effect over an area. This effect can be represented by the weighting functions $g_i(x,y)$. The relation between these functions is:

$$\Delta Q(x,y) = \lambda_i g_i(x,y) \qquad (5.24)$$

The gradient of the criterion $J(\lambda 1,\ldots,\lambda m)$ can now be written as:

$$\frac{\partial J}{\partial \lambda_i} = \sum_{x \in D} \frac{\partial J}{\partial Q(x,y)} g_i(x,y) \qquad (5.25)$$

For the rectangular or triangular method used in WAQAD $g_i(x,y)$ is 0 or 1 and the gradient is just the summation over the rectangle. If one looks at the way the gradient is computed with the adjoint method, the summation (5.25) already forms a natural part of the computation. All that needs to be done is to save all the required information. The situation when one

wants to split the gradient in time is a little more intricate, but the solution is almost the same and again all that needs to be done is to store the required information.

Filtering the data

The raw data obtained by storing the information during the computations of the adjoint model have a regular part and some high frequency irregularities or noise. A discrete time filter is used to obtain a smoother picture. The only parameter needed for the filter is the cut-off frequency. Most of the noise has a frequency close to the one corresponding to the time between the data. The input should be given as a fraction of the Nyquist frequency; this means that if one is given as an input, all frequencies are passed and output data is the same as input data. A good indication of this fraction is the inverse of the number of simulation steps between two time steps with measurement data.

Let a(k) be a series of data then the Fourier transform is given by:

$$\hat{a}(\omega) = \sum_{k} e^{-i\omega k} a(k)$$

and the inverse transform is given by:

$$a(k) = \int_{-\pi}^{\pi} \frac{1}{2\pi} e^{i\omega k} \hat{a}(\omega) d\omega$$

If we cut off all the frequencies above ω_0 then the Fourier transform of this filtered data $\hat{b}$ becomes:

$$\hat{b}(\omega) = \begin{cases} a(\omega) ; \omega \le \omega_0 \\ 0 \quad ; \omega > \omega_0 \end{cases}$$

In the time domain this transformation can be described by the convolution:

$$b(k) = \sum_{l} g(l)a(k-l)$$

where g can be shown to be:

$$g(l) = \begin{cases} \dfrac{\omega_0}{\pi} & ; l = 0 \\ \dfrac{1}{\pi l}\sin(\omega_0 l) & ; l \neq 0 \end{cases}$$

This is for infinitely long series. For finite series the truncated convolution is divided by the sum of the corresponding g(l).

In two dimensions the problem can be solved analogously, but it becomes slightly more difficult to handle of all exceptions becomes.

5.4.3. Implementation

Several programs are used at RIKZ for more common variables like water levels. None of these programs is currently able to cope with the new variables introduced in this section.

After comparing various alternatives a sequence of two programs was chosen. First the data file is read with a FORTRAN program and the filtered data are written to an ASCII file. In the second step a script written in MATLAB language is used to plot the pictures to the screen or the printer.

When this program is started a menu appears on the screen and the user can use the mouse to select plots and analyse the data. More than one window for plots can be used at the same time and several plots can be displayed in one window. Also a number of options for the presentation of the data are offered.

At the moment the FORTRAN program ADPIC is fully implemented. There is also a working test version VIZ of the MATLAB script. See the WAQAD User's Guide, for more information on the ADPIC and VIZ programs.

5.4.4. Practical use and interpretation of results

The extensions described in this section can be used in several ways. Probably the most important use is to depict the spatial gradient for depth and bottom friction to select rectangles (or triangles) for the optimization process. Using these depictions the situation in which a non-zero gradient cancels over a selected rectangle can be avoided. This is important since a zero gradient leads to no adaptation, while the criterion can still be lowered using other triangles. Furthermore, the magnitude of the gradient in space gives an indication of the sensitivity of the criterion to changes and it is probably possible to make a detailed estimation of the parameter. In areas where the gradient is small a detailed estimation is probably not possible and larger rectangles should be selected. The application of these rules is shown in an example in [Verlaan, 1994].

Another application is to use the gradient as a function of time for the selection of the simulation period. The actual gradient used in the minimization procedure is the average over time of the function. This average corresponds to the mean of the function. Usually the function will show deviations from this average in time. The random fluctuations show the propagation of the noise and indicate if the time interval is long enough to obtain a sufficiently accurate estimate of the gradient. The systematic fluctuations indicate model imperfections. If these systematic fluctuations change in time it is important for the interval used for calibration to be a good reflection of the interval that will be used with the model for prediction. If the model is to be used to predict tidal maxima and minima, for example, and there is in spring tide and neap tide fluctuation in the gradient, then the interval for calibration should be a month or a multiple of a month. These effects are illustrated with some examples in [Verlaan, 1994].

5.4.5. Use of the Hessian

Together with the normal output of the program, the Hessian and its eigenvalues are given (see subsection 5.1.4). The Hessian, the matrix of all second derivatives, gives us information on the 'shape' of the surface of the criterion at the (local) minimum. From maximum likelihood theory it can be shown that the inverse of the Hessian converges to the a posteriori covariance of the parameters, and thus the inverse Hessian can be used to give an error bound to the estimate. The estimate of the inverse Hessian should be used with care. Only when the estimate converges to the 'true' parameter is it certain that the covariance is correct. If this is the case, the error of the parameters will be asymptotically normal, and all kinds of tests may then be used.

The estimate of the inverse Hessian is generated by the second order algorithm that is used in the minimization. This algorithm only gives an accurate estimate in the limit. In practice the result is often close to the limiting result after a number of iterations equal to the number of parameters plus one. This result implies that in order to use the inverse Hessian estimate for error bounds on the estimate of the parameters, the number of iterations should be large enough for the convergence of this estimate.

Another and probably more important use of the inverse Hessian is to detect problems in the estimation problem. When the problem specified by the user has almost the same value of the criterion for some parameter in neighborhood it is not possible to give accurate estimates for the parameters, see also subsection 5.1.4.

5.4.6. Conclusions

The gradient of the criterion used in WAQAD for estimating parameters can be split either in time or in space. The resulting functions can be used to analyse the model. They can also be useful in selecting the parameters for the input of WAQAD, but additional experience is needed to make this a practical and reliable procedure.

Programs ADPIC and VIZ were designed and implemented to produce plots of these functions. It is currently possible to make plots of the gradients of bottom friction, depth, vertical viscosity and boundary components for every model that runs under WAQAD for SIMONA.

5.5. The use of current velocity measurements

Velocity measurements can be of great use for the calibration of models. If, for instance, the model is going to be used to compute sediment or pollution transport, the current velocity is very sensitive to the tidal average of the water level that is prescribed at the boundary. If only measurements of the water level are available and the average water level at the boundary is to be calibrated, the problem can be very ill conditioned. To illustrate this, assume no tide is present and the effect is dominated by the following part of the shallow water equations in one dimension:

$$g\frac{\partial \zeta}{\partial x} + \frac{gu^2}{C^2 H} = 0$$

Two observations can be made from this equation. The velocity is highly dependent on the bottom friction value, which is not known very accurately and also the velocity is very sensitive to the difference in water level between two points. Substituting the values C=50[s^2m^{-1}], H=10[m] then a 10% change in the average velocity (u=0.1[m^{s-1}] to u=0.11[ms^{-1}]) corresponds to a difference of $\delta h/\delta x$ of about one centimetre per 100 kilometres. This kind of accuracy is very difficult to obtain with water level measurements, and current velocity measurements can greatly improve the performance of the calibration.

In general, automatic calibration performs best when as many reliable measurements as possible are included, since all other variables in the model will have to be guessed from the available measurements and the model, which sometimes means that variables for which no measurements are available will not be accurate.

[Verlaan, 1994] describes in detail extending WAQAD to use velocity measurements. However, this extension has not yet been implemented in WAQAD. Research is currently in progress on using velocity measurements in a separate test version of WAQAD, see [Mooij, 1996].

5.6. Friction formulations

5.6.1. Introduction

The friction term is an important part of the two- and three-dimensional shallow water equations. It is very indirectly related to physical concepts. Very briefly the origin of this term can be described as follows.

Basically the shallow water equations, as approximated by WAQUA-in-SIMONA, originate from Newton's law, F=MA, and the conservation of mass. In the presence of viscosity the flow becomes turbulent for higher Reynold numbers. Since finite difference methods, as used in WAQUA-in-SIMONA, can only compute smooth solutions a direct solution of the turbulent flow is impossible. Often one is only interested in the average flow and not in the turbulent fluctuations. In this case it is possible to average the equation over a time interval to obtain time-averaged flow. In the process of averaging, new terms are created that represent the turbulent energy. To obtain a closed set of equations an assumption about this energy has to be made. Often this is in the form of diffusion approximation. To obtain two-dimensional, depth-averaged, equations the equations resulting from the process above are averaged over the vertical coordinate from bottom to surface. This integration introduces a number of new terms one of which is the stress (turbulent and viscous) on the bottom. A new assumption has to be made here to obtain a closed set of equations. The bottom stress is often assumed to be directed opposite to the depth averaged flow and proportional to the square of the magnitude. In the past, measurements have indicated that the friction depends on the local water depth, and several empirical (or mainly empirical) formulas for this dependence are widely used, especially the Chezy, Manning and White-Colebrook formulations.

In WAQUA-in-SIMONA one of these three formulations for the dependence of friction on the local water depth has to be chosen. Since all three formulations contain a parameter (usely known), the calibration procedure should be able to deal with all three types of parameters.

The Chezy formulation had already been implemented in WAQAD. The friction terms in this documentation (in chapters 3 and 4) were therefore described for the Chezy formulations. Recently, the WAQAD system was extended to use Manning and White-Colebrook formulations too. In this section the extension of WAQAD to the other formulations is described.

5.6.2. Theoretical background

For a detailed theoretical derivation of the friction formulations, see [Verlaan, 1994]. In this section the derivation of the friction formulations is described briefly, since part of the derivation in [Verlaan, 1994] has already been described in chapters 3 and 4 of this documentation.

The friction terms for the Chezy formulation are given by equations (3.11) and (3.14):

$$fruu_{m,n} = \frac{g}{C_u^2} \frac{2(u_{m,n})^2 + (\overline{v}^{\eta\xi}_{m,n})^2}{H^u \sqrt{(u_{m,n})^2 + (\overline{v}^{\eta\xi}_{m,n})^2}}$$

$$fruv_{m,n} = \frac{g}{C_u^2} \frac{u_{m,n}\, \overline{v}^{\eta\xi}_{m,n}}{H^u \sqrt{(u_{m,n})^2 + (\overline{v}^{\eta\xi}_{m,n})^2}}$$

$$fruwl_{m,n} = -\frac{g}{C_u^2} \frac{u_{m,n} \sqrt{(u_{m,n})^2 + (\overline{v}^{\eta\xi}_{m,n})^2}}{(H^u)^2}$$

$$frvu_{m,n} = \frac{g}{C_v^2} \frac{\overline{u}^{\xi\eta}_{m,n}\, v_{m,n}}{H^v \sqrt{(\overline{u}^{\xi\eta}_{m,n})^2 + (v_{m,n})^2}}$$

$$frvv_{m,n} = \frac{g}{C_v^2} \frac{(\overline{u}^{\xi\eta}_{m,n})^2 + 2(v_{m,n})^2}{H^v \sqrt{(\overline{u}^{\xi\eta}_{m,n})^2 + (v_{m,n})^2}}$$

$$frvwl_{m,n} = -\frac{g}{C_v^2} \frac{v_{m,n} \sqrt{(\overline{u}^{\xi\eta}_{m,n})^2 + (v_{m,n})^2}}{(H^v)^2}$$

In these formulations C is the Chezy coefficient, where Cu is defined at a u point and Cv at a v point. For the other friction formulations coefficient C has a different dependence on H:

- Chezy formulation:

  $C = constant$

- Manning formulation:

  $$C = \frac{H^{\frac{1}{6}}}{M}$$

  where M is Manning's parameter.

- White-Colebrook formulation:

$$C = 18\log(\max(\frac{12H}{W}, 1.0129))$$

where W is the White-Colebrook parameter.

The coefficients fruu, fruv, frvu and frvv do not depend on the friction formulation chosen. The coefficients fruwl and frvwl, however, do depend on the friction formula, since they depend on the total water depth H. For the Manning and White-Colebrook formulation they become:

- Manning:

$$fruwl_{m,n} = \frac{4}{3}\frac{-g}{C_u^2}\frac{u_{m,n}\sqrt{(u_{m,n})^2 + (\overline{v}^{\eta\xi}_{m,n})^2}}{(H^u)^2}$$

$$frvwl_{m,n} = \frac{4}{3}\frac{-g}{C_v^2}\frac{v_{m,n}\sqrt{(\overline{u}^{\xi\eta}_{m,n})^2 + (v_{m,n})^2}}{(H^v)^2}$$

- White-Colebrook:

$$fruwl_{m,n} = \left(1 + \frac{36}{C_u \ln 10}\right)\frac{-g}{C_u^2}\frac{u_{m,n}\sqrt{(u_{m,n})^2 + (\overline{v}^{\eta\xi}_{m,n})^2}}{(H^u)^2}$$

$$frvwl_{m,n} = \left(1 + \frac{36}{C_v \ln 10}\right)\frac{-g}{C_v^2}\frac{v_{m,n}\sqrt{(\overline{u}^{\xi\eta}_{m,n})^2 + (v_{m,n})^2}}{(H^v)^2}$$

for $H > \frac{1.0129}{12} W$, and equal to the friction formulation for Chezy otherwise.

The gradient for the bottom friction also changes according to the adaptations resulting from the friction formulations. For a detailed derivation the reader is again referred to [Verlaan, 1994] and [Brouwer, 1995c]. Table 5.1 shows how the gradient changes as a result of other friction formulations:

friction formulation	**absolute**	**percentual**
Chezy	$\frac{grc}{C}$	grc
Manning	$\frac{grc}{C}\frac{-.75C}{M} = \frac{-.75grc}{M}$	-.75grc
White-Colebrook	$\frac{grc}{C}\frac{1}{1+\frac{36}{C\ln 10}}\frac{-18}{W\ln 10} = \frac{-grc}{w\left(c\frac{\ln 10}{18}+2\right)}$	$\frac{-grc}{C\frac{\ln 10}{18}+2}$

table 6.3 Adaptations of the bottom friction gradient as a result of other friction formulations

where:

- grc is the bottom friction gradient:
  $grc = (\nu_u)2H^u\,fruwl$
  in u points and
  $grc = (\nu_v)2H^v\,frvwl$
  in v points.
- The percentual gradient is calculated by:
  <percentual grad> = <absolute grad> * <friction>
- The adaptations according to White-Colebrook are only calculated if
  $H > \frac{1.0129}{12}W$.

5.6.3. Implementation

According to other friction formulations the coefficients fruu, fruv, frvu and frvv do not change. However, the coefficients fruwl and frvwl do change; they acquire an additional factor:

- Manning : $\frac{4}{3}$
- White-Colebrook : $1+\frac{36}{C\ln 10}$ if $H > \frac{1.0129}{12}W$ and 1 otherwise.

The changes in the gradient resulting from the friction formulations are described by the factors shown in table 6.1.

These extensions for Manning and White-Colebrook friction formulations are implemented in WAQAD. For more information on this implementation, see [Brouwer, 1995c].

5.7. Finite difference calculations

Models can be calibrated by selecting input parameters which may be adapted in such a way that the prediction results are the best possible. The square mean of the error (error = prediction - observation) is usually chosen as the critirion for the prediction value. A certain input parameter can be adapted using steps of different sizes. For each step a simulation is run and the corresponding prediction value is calculated. In this way a number of points are calculated with X=step size and Y=prediction value. These points form the cost function of the corresponding parameter to be calibrated.

The cost function is parabolic. A model is calibrated by searching for the minimum of the cost function of the selected input parameter. This minimization is carried out by calculating the gradient (=direction coefficient of the tangent of the parabola for X=0.) for each parameter, after which a search process is started. During this search a number of simulations are run with different step sizes for the adaptions of the parameter in the direction of the gradient. This is done until the minimum with the required accuracy is determined.

There are different methods for calculating the gradient. Using the adjoint model it is possible to determine the complete gradient vector for an undetermined number of parameters in one simulation run. This method, on which WAQAD is based, is fully described in this documentation.

Finite difference is the 'classical' method for calibrating models. The minimization of this method shows the same iterative progress as WAQAD, except that the gradient is calculated differently. WAQAD calculates the gradient for each selected parameter in one single adjoint simulation run. Using the finite difference method a WAQUA simulation run must be started for each selected parameter in order to determine the gradient.

Using the finite difference method the gradient of a selected parameter is calculated as follows:

- Determine value J0 of the cost function of the initial WAQUA run (see the WAQAD User's Guide for calculation of the cost function).
- Adapt the values of the selected parameters with a prescribed value S and determine the value J1 of the cost function of the WAQUA run with adapted input.
- Calculate the gradient: G=(J0-J1)/S.

Step size S must be chosen small enough so that gradient G approximates the direction coefficient of the parabola. However, if the step size is too small, problems of machine

accuracy may occur. In order to be able to calculate a reliable gradient using the finite difference method, some research must be performed on the shape of the parabola.

WAQAD offers the possibility of calculating the gradient by using either the adjoint method or the finite difference method. The latter method has one advantage:

- It can be used to check the gradient calculation of the adjoint method, by checking the correctness of the implementation when new types of parameters are introduced, such as vertical viscosity or salinity.

The finite difference method will mainly be used as control tool or to investigate if it is useful to calibrate a certain type of parameter. Its use as a calibration tool is not advised, for the following reasons:

- The gradient cannot be calculated exactly. During every iteration the shape of the cost function for each parameter must be searched in order to get an indication of the step size to be used.

- The computational time required is dependent on the number of parameters. In addition to an initial WAQUA run, a WAQUA run for each parameter is required in order to calculate the gradient. This in contrast with the adjoint method, which only requires one single adjoint run in order to calculate the complete gradient vector.

For more information on using the finite difference method, see [Brouwer, 1995b].

5.8. Velocity and discharge boundaries

Until recently WAQAD was only able to recognize closed and open water level boundaries. Open velocity and discharge boundaries were treated as open water level boundaries. Because of this, the velocities prescribed by WAQUA at open boundaries were treated in the adjoint model equations as if they were velocities in the interior field. This 'wrong' approach has been corrected in WAQAD in order to gain completeness. Thus open boundaries are now treated by WAQAD in the following way:

- If an open boundary is a water level boundary, then the water level points at this boundary do not take part in the adjoint calculation. The nearest neighbour velocity points do take part in the adjoint calculation.
- If an open boundary is not a water level boundary but a velocity or discharge boundary, then the water level points and the velocity points at the boundary do not take part in the adjoint calculation.

For more information on the implementation of velocity and discharge boundaries, see [Brouwer, 1995b].

6. Recommendations

Remarks on WAQAD with respect to WAQUA and TRIWAQ were made in chapters 3 and 4 respectively. An overview of these remarks is listed below:

- The WAQAD bottom friction terms contain a shift of half a time step compared with the bottom friction terms in WAQUA.

- Horizontal viscosity is not included in WAQAD, both for 2D and 3D models.

- Horizontal advection is not included in WAQAD in the case of 3D models.

- The horizontal advection terms are solved in WAQUA using the Gauss-Seidel method. In WAQAD these horizontal advection terms are solved using a Jacobi method.

- Additional WAQUA and TRIWAQ features are not included in WAQAD. The features of concern are:
  - External forcings like wind, discharges and density gradient.
  - Transports, STRESS2d, barriers and weirs.
  - Smoothing boundary values.
  - Depth multiplier.

- In TRIWAQ there are two ways to prescribe layers: fixed layers or sigma layers. WAQAD assumes that no fixed layers are prescribed in the forward model.

In the past, more differences existed between WAQAD and WAQUA. For example, horizontal advection was not a feature of WAQAD. But when the horizontal advection was also included in WAQAD, the calibration process really improved. It is expected that WAQAD will perform better if other missing features are assimilated too. Therefore, it is recommended that:

- WAQAD is fully consistent with WAQUA and TRIWAQ.

Furthermore, it is recommended that:

- WAQAD is extended to the use of water velocity measurements. This has already been tested by means of a special test version of WAQAD, see [Mooij, 1996]. The results are promising.

- WAQAD is extended to estimate the standard deviations of the measurements. In theory it is possible to use the Maximum Likelihood method to determine the optimal standard deviations of the measurements. The ability to estimate these standard deviations automatically would also reduce the number of parameters that the user has to specify. However, this estimation is computationally somewhat different from the other parameters, but not trivial: the derivation is much more complex. Experiments will be needed to determine the usefulness of this procedure, since it can become instable.

- To implement the possibility of producing warnings if the estimation procedure does not work properly, e.g. if the problem is not identifiable. This information can be obtained from the Hessian, the standard deviations and the value of the criterion. The automatic detection of these kinds of problems could save many hours of waiting for a result that then shows that the input was wrong.

7. Appendices

7.1. Documenthistory

Version	Date	Description
1.0a	June 3, 1996	Concept
1.0	October 25, 1996	First edition

7.2. References

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7.3. List of symbols

$.'$ = variable at time t+½Δt

$.''$ = variable at time t+Δt

$.^{-'}$ = variable at time t-½Δt

ζ = water elevation above plane of reference

ζ_0 = averaged sea surface

$\overline{\zeta}^{\eta}$ = $\frac{1}{2}[\zeta_{m,n}+\zeta_{m,n+1}]$

$\overline{\zeta}^{\xi}$ = $\frac{1}{2}[\zeta_{m,n}+\zeta_{m+1,n}]$

$\zeta_{0\eta}$ = $\dfrac{\zeta_{n+1}-\zeta}{\Delta\eta}$

$\zeta_{0\xi}$ = $\dfrac{\zeta_{m+1}-\zeta}{\Delta\xi}$

ξ, η = horizontal curvilinear coordinates

$\Delta\eta$ = grid distance in η direction

$\Delta\xi$ = grid distance in ξ direction

(ν_ζ) = adjoint water level

$(\nu_\zeta)_{0\eta}$ = $\dfrac{(\nu_\zeta)_{n+1}-(\nu_\zeta)}{\Delta\eta}$

$(\nu_\zeta)_{0\xi}$ = $\dfrac{(\nu_\zeta)_{m+1}-(\nu_\zeta)}{\Delta\xi}$

$\overline{(\nu_\zeta)}^{\eta}$ = $\frac{1}{2}\left[\,(\nu_\zeta)+(\nu_\zeta)_{n+1}\,\right]$

$\overline{(\nu_\zeta)}^{\xi}$ = $\frac{1}{2}\left[\,(\nu_\zeta)+(\nu_\zeta)_{m+1}\,\right]$

(ν_u) = adjoint velocity in x direction

$(\nu_u)_{0\xi}$ = $\dfrac{(\nu_u)-(\nu_u)_{m-1}}{\Delta\xi}$

$\overline{(\nu_u)}^{\xi\eta}$ = $\overline{\overline{(\nu_u)}^{\xi}}^{\eta}$

= $\frac{1}{4}\left[\,(\nu_u)+(\nu_u)_{n+1}+(\nu_u)_{m-1,n+1}+(\nu_u)_{m-1}\,\right]$

(ν_v) = adjoint velocity in y direction

$(\nu_v)_{0\eta}$ = $\dfrac{(\nu_v)-(\nu_v)_{n-1}}{\Delta\eta}$

$\overline{(\nu_v)}^{\eta\xi}$ = $\overline{\overline{(\nu_v)}^{\eta}}^{\xi}$

= $\frac{1}{4}\left[\,(\nu_v)+(\nu_v)_{n-1}+(\nu_v)_{m+1,n-1}+(\nu_v)_{m+1}\,\right]$

ν_v = vertical viscosity coefficient

$\delta_z(\,w\delta_z u')$ = $\dfrac{1}{h}\left[\,\overline{\nu_V}^{\xi}\,\dfrac{u'_{k-1}-u'}{\frac{1}{2}(h_{k-1}+h)}-\overline{\nu_V}^{\xi}\,\dfrac{u'-u'_{k+1}}{\frac{1}{2}(h+h_{k+1})}\,\right]$

$\delta_z(\,w\delta_z v')$ = $\dfrac{1}{h^V}\left[\,\overline{\nu_V}^{\eta}\,\dfrac{v'_{k-1}-v'}{\frac{1}{2}(h^V_{k-1}+h^V)}-\overline{\nu_V}^{\eta}\,\dfrac{v'-v'_{k+1}}{\frac{1}{2}(h^V+h^V_{k+1})}\,\right]$

ϕ = phase of harmonic constituent

ω = angular velocity of harmonic constituent

A = amplitude of harmonic constituent
C = chezy coefficient for model bottom roughness
d = water depth below plane of reference
D^u = D^{ξ}
= $\frac{1}{2}(d_{m,n}+d_{m,n-1})$
D^v = D^{η}
= $\frac{1}{2}(d_{m-1,n}+d_{m,n})$
E = distance between depth points in η direction
= $guu = \sqrt{g_{\eta\eta}}$, the WAQUA transformation coefficient
$E^{\xi}_{m,n}$ = $\frac{1}{2}(E_{m-1,n}+\zeta_{m,n})$
E^v = $\bar{E}^{\xi\eta}$
= $\frac{1}{4}(E_{m-1,n}+E_{m,n}+E_{m,n+1}+E_{m-1,n+1})$
f = Coriolis force
fruu = bottom friction contribution in u velocity point to the adjoint u momentum equation

$$= \frac{g}{C_u^2}\frac{2(u_{m,n})^2+(\bar{v}^{\eta\xi}_{m,n})^2}{(D^u_{m,n}+\bar{\zeta}^{\xi}_{m,n})\sqrt{(u_{m,n})^2+(\bar{v}^{\eta\xi}_{m,n})^2}}$$

fruv = bottom friction contribution in u velocity point to the adjoint v momentum equation

$$= \frac{g}{C_u^2}\frac{u_{m,n}\,\bar{v}^{\eta\xi}_{m,n}}{(D^u_{m,n}+\bar{\zeta}^{\xi}_{m,n})\sqrt{(u_{m,n})^2+(\bar{v}^{\eta\xi}_{m,n})^2}}$$

fruwl = bottom friction contribution in u velocity point to the adjoint continuity equation

$$= -\frac{g}{C_u^2}\frac{u_{m,n}\sqrt{(u_{m,n})^2+(\bar{v}^{\eta\xi}_{m,n})^2}}{(D^u_{m,n}+\bar{\zeta}^{\xi}_{m,n})^2}$$

frvu = bottom friction contribution in v velocity point to the adjoint u momentum equation

$$= \frac{g}{C_v^2}\frac{\bar{u}^{\xi\eta}_{m,n}\,v_{m,n}}{(D^v_{m,n}+\bar{\zeta}^{\eta}_{m,n})\sqrt{(\bar{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}}$$

frvv = bottom friction contribution in v velocity point to the adjoint v momentum equation

$$= \frac{g}{C_v^2}\frac{(\bar{u}^{\xi\eta}_{m,n})^2+2(v_{m,n})^2}{(D^v_{m,n}+\bar{\zeta}^{\eta}_{m,n})\sqrt{(\bar{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}}$$

frvwl = bottom friction contribution in v velocity point to the adjoint continuity equation

$$= -\frac{g}{C_v^2}\frac{v_{m,n}\sqrt{(\bar{u}^{\xi\eta}_{m,n})^2+(v_{m,n})^2}}{(D^v_{m,n}+\bar{\zeta}^{\eta}_{m,n})^2}$$

$fruu^{3D}$ = $\frac{g}{C_u^2}\frac{2(u_K)^2+(\bar{v}^{\eta\xi}_K)^2}{h_K\sqrt{(u_K)^2+(\bar{v}^{\eta\xi}_K)^2}}$

$fruv^{3D}$ = $\frac{g}{C_u^2}\frac{u_K\,\bar{v}^{\eta\xi}_K}{h_K\sqrt{(u_K)^2+(\bar{v}^{\eta\xi}_K)^2}}$

$frvu^{3D}$ = $\frac{g}{C_v^2}\frac{\overline{u_K^{\xi\eta}}\,v_K}{h_K^v\sqrt{(\overline{u_K^{\xi\eta}})^2+(v_K)^2}}$

$frvv^{3D}$ = $\frac{g}{C_v^2}\frac{(\overline{u_K^{\xi\eta}})^2+2(v_K)^2}{h_K^v\sqrt{(\overline{u_K^{\xi\eta}})^2+(v_K)^2}}$

$frwl^{3D}$ = $\frac{g}{C^2}\frac{u'_K\sqrt{(u'_K)^2+\left(\overline{v_K}^{\xi\eta}\right)^2}}{(h_K)^2}\frac{v'_k\sqrt{(v_K)^2+\left(\overline{u'_K}^{\xi\eta}\right)^2}}{(h_K^v)^2}$

$+\frac{g}{C^2}\frac{v'_K\sqrt{(v_K)^2+\left(\overline{u'_K}^{\xi\eta}\right)^2}}{(h_K^v)^2}$

F = external force

g = acceleration of gravity

h = layer thickness

H = total water depth (d + ζ)

$(H^u)_{m,n}$ = H^{ξ}

= $\frac{1}{2}(\zeta_{m,n}+\zeta_{m+1,n}+d_{m,n}+d_{m,n-1})$

$(H^v)_{m,n}$ = H^{η}

= $\frac{1}{2}(\zeta_{m,n}+\zeta_{m,n+1}+d_{m-1,n}+d_{m,n})$

k = layer index

K = distance between depth points in ξ direction

= gvv = $\sqrt{g_{\xi\xi}}$, the WAQUA transformation coefficient

$K^{\eta}_{m,n}$ = $\frac{1}{2}(K_{m,n-1}+K_{m,n})$

$K^{u}_{m,n}$ = $\overline{K}^{\eta\xi}$

= $\frac{1}{4}(K_{m,n-1}+K_{m+1,n-1}+K_{m+1,n}+K_{m,n})$

m = horizontal grid index in m direction

n = horizontal grid index in y direction

t = time

Δt = integration timestep

u = horizontal velocity component in x direction

$\overline{u}^{\xi}$ = $\frac{1}{2}\left[u_{m-1}+u\right]$

$u_{0\xi}$ = $\frac{u-u_{m-1}}{\Delta\xi}$

$\overline{u}^{\xi\eta}$ = $\overline{\overline{u}^{\xi}}^{\eta}$

= $\frac{1}{4}\left[\,u+u_{n+1}+u_{m-1,n+1}+u_{m-1}\,\right]$

$\overline{\overline{u}}$ = $\overline{\overline{u}^{\xi}}^{\eta}$

U = depth averaged horizontal velocity component in x direction

U = $\frac{1}{H}\sum_{k=1}^{K}u\,h$

= $\frac{U-U_{m-1}}{\Delta\xi}$

v = horizontal velocity component in y direction

$\bar{v}^{\eta}$ = $\frac{1}{2}\left[v_{n-1} + v\right]$

$v_{0\eta}$ = $\frac{v - v_{n-1}}{\Delta\eta}$

$\bar{v}^{\eta\xi}$ = $\overline{\bar{v}^{\eta}}^{\xi}$

= $\frac{1}{4}\left[v + v_{n-1} + v_{m+1,n-1} + v_{m+1}\right]$

$\bar{\bar{v}}$ = $\overline{\bar{v}^{\eta}}^{\xi}$

V = depth averaged horizontal velocity component in y direction

= $\frac{1}{H}\sum_{k=1}^{K} vh^{v}$

$V_{0\eta}$ = $\frac{v - v_{n-1}}{\Delta\eta}$

z_k = position of layer interface

7.4. Advection in the case of bounderies and dryfall

Up till now we assumed that no degenerations take place in the discretization of the advective terms in WAQUA, although this discretization depends on the dry/wet status of surrounding points. In fact it was assumed that the surrounding points were all wet. The presence of boundaries and the dryfall procedure are responsible for the deformations of the advective terms. These alterations have consequences for the adjoint advective terms in the inverse model. That is the subject of this appendix.

7.4.1. Closed Boundaries

Closed boundaries are land-water boundaries. These are represented by zero velocities in either the x- or y direction. Due to the drying and flooding procedure this geometric information varies with time. We are going to examine the influence of impeded geometry on the numerical treatment of the advective term uu_x in the computational procedures of WAQUA. Firstly, we consider the alterations in the adjoint u impulse equation associated with $\Delta u'_{m,n}$.

- Degenerations in the adjoint u impulse equation associated with $\Delta u'_{m,n}$ caused by impeded geometry.

An array GEOUUX is constructed from which the time-dependent local flow situation can be determined. In WAQUA impeded u velocity points are denoted by KHU ≤ 0 (0 for permanent dry and -1 for temporary dry). These variables are part of the 'solution flow' and may change from time to time.

KHU(m-1,n)	KHU(m,n)	KHU(m+1,n)	GEOUX(m,n)
>0	>0	>0	1: central
>0	>0	≤ 0	2: upwind
≤ 0	>0	>0	3: upwind
other			0: no advection

Table I Definition of array GEOUUX

The situation GEOUUX = 1 is already handled in section 3.2.2. This is the case were the surrounding points are wet. Than, a central difference is used to approximate u_x, otherwise a first order upwind scheme or zero. This information is important for the construction of the adjoint

advective terms, since there is a one-to-one relationship between WAQUA and its inverse model.

- GEOUUX(m,n) = 2. In this case the term uu_x is discretized at the first stage as:

$$u'_{m,n}\,\frac{\left(u_{m,n}-u_{m-1,n}\right)}{\Delta X},\ \text{if}\ u_{m,n}>0 \tag{7.1}$$

Introducing Lagrange multipliers and applying variational formalism yields:

$$(\nu_u)'_{m,n}\left\{\cdots\Delta u'_{m,n}\,\frac{\left(u_{m,n}-u_{m-1,n}\right)}{\Delta X} + u'_{m,n}\,\frac{\left(\Delta u_{m,n}-\Delta u_{m-1,n}\right)}{\Delta X}\cdots\right\} \tag{7.2}$$

At the second stage as:

$$u'_{m,n}\,\frac{\left(u''_{m,n}-u''_{m,n}\right)}{\Delta X},\ \text{if}\ u'_{m,n}>0 \tag{7.3}$$

Introducing Lagrange multipliers and applying variational formalism yields:

$$(\nu_u)''_{m,n}\left\{\cdots\Delta u'_{m,n}\,\frac{\left(u''_{m,n}-u''_{m-1,n}\right)}{\Delta X} + u'_{m,n}\,\frac{\left(\Delta u''_{m,n}-\Delta u''_{m-1,n}\right)}{\Delta X}\cdots\right\} \tag{7.4}$$

- GEOUUX(m,n) = 3. In this case the term uux is discretized at the first stage as:

$$u'_{m,n}\,\frac{\left(u_{m+1,n}-u_{m,n}\right)}{\Delta X},\ \text{if}\ u_{m,n}\le 0 \tag{7.5}$$

Introducing Lagrange multipliers and applying variational formalism yields:

$$(\nu_u)'_{m,n}\left\{\cdots \Delta u'_{m,n}\frac{\left(u_{m+1,n}-u_{m,n}\right)}{\Delta X} + u'_{m,n}\frac{\left(\Delta u_{m+1,n}-\Delta u_{m,n}\right)}{\Delta X}\cdots\right\} \tag{7.6}$$

At the second stage as:

$$u'_{m,n}\frac{\left(u_{m+1,n}-u''_{m,n}\right)}{\Delta X},\ \text{if}\ u'_{m,n}\le 0 \tag{7.7}$$

Introducing Lagrange multipliers and applying variational formalism yields:

$$(\nu_u)''_{m,n}\left\{\cdots \Delta u'_{m,n}\frac{\left(u''_{m+1,n}-u''_{m,n}\right)}{\Delta X} + u'_{m,n}\frac{\left(\Delta u''_{m+1,n}-\Delta u''_{m,n}\right)}{\Delta X}\cdots\right\} \tag{7.8}$$

It follows that the adjoint u impulse equation associated with $\Delta u'_{m,n}$ solved in procedure AD-SUV (boundary effects and dryfall and advective terms included) looks like:

- Determine for all u velocity points the array GEOUUX (Table I) at time t+½Δt.

$$\boxed{(\nu_u)'_{m,n}} = DD_{m+1,n} - CC_{m+1,n}\left[\ \boxed{(\nu_h)'_{m+,n}} - \boxed{(\nu_\zeta)'_{m,n}}\ \right] \qquad (7.9)$$

with:

$$CC_{m+1,n} = \frac{-(H^u)'_{m,n}}{\Delta X\left[\ \frac{2}{\Delta t} + fruu'_{m,n} + AU1\ \right]}$$

$$DD_{m+1,n} = \frac{\left[\ \frac{2}{\Delta t} - fruu'_{m,n} - AU1D\ \right](\nu_u)''_{m,n}}{\left[\ \frac{2}{\Delta t} + fruu'_{m,n} + AU1\ \right]}$$

$$- \frac{(H^u)'_{m,n}\left[(\nu_\zeta)''_{m,n} - (\nu_\zeta)''_{m+1,n}\right]}{\Delta X\left[\ \frac{2}{\Delta t} + fruu'_{m,n} + AU1\ \right]}$$

- If GEOUUX(m,n) = 1:

$$AU1 = \frac{\left(u_{m+1,n} - u_{m-1,n}\right)}{2\Delta X} \qquad (7.10)$$

$$AU1D = \frac{\left(u''_{m,n} - u''_{m-1,n}\right)}{2\Delta X}$$

- If GEOUUX(m,n) = 2: (7.11)

$$AU1 = \frac{\left(u_{m,n} - u_{m-1,n}\right)}{\Delta X},\ \text{if } u_{m,n} > 0$$
$$= 0,\ \text{otherwise}$$

$$AU1D = \frac{\left(u''_{m,n} - u''_{m-1,n}\right)}{\Delta X},\ \text{if } u'_{m,n} > 0$$
$$= 0,\ \text{otherwise}$$

- If GEOUUX(m,n) = 3: (7.12)

$$AU1 = \frac{\left(u_{m+1,n} - u_{m,n}\right)}{\Delta X},\ \text{if } u_{m,n} \le 0$$
$$= 0,\ \text{otherwise}$$

$$AU1D = \frac{\left(u''_{m+1,n} - u''_{m,n}\right)}{\Delta X},\ \text{if } u'_{m,n} \le 0$$
$$= 0,\ \text{otherwise}$$

So far, we handled the degenerations in the adjoint advective terms caused by impeded points in the adjoint u impulse equation. In the next part we focus on the deformations of the second order difference operator S^c and S^u.

•• Degenerations in the adjoint v impulse equation associated with $\Delta v'_{m,n}$ caused by impeded geometry.

In the adjoint v impulse equation associated with $\Delta v'_{m,n}$ the second order difference operators S^c (central) and S^u (upwind) appear. In this appendix the boundary treatment of these operators in the adjoint computation process is indicated. These approximations depend on the dry/wet status of the surrounding points. Therefore, the (time-dependent) local flow situation has to be determined first to figure out which approximation has been used in the computation process of WAQUA.

- $S^c_y(u_{m,n})$ and $S^u_y(u''_{m,n})$

We define for each u velocity point the logical variables (True or False) KBB, KB, KT and KTT with which the arrays GEBVUY and GETVUY are determined.

KBB(m,n) = KHV(m,n-2) > 0 $\wedge$ KHU(m,n-2) > 0 $\wedge$ KHV(m+1,n-2)> 0

KB(m,n) = KHV(m,n-1) > 0 $\wedge$ KHU(m,n-1) > 0 $\wedge$ KHV(m+1,n-1)> 0

KT(m,n) = KHV(m,n) > 0 $\wedge$ KHU(m,n+1) > 0 $\wedge$ KHV(m+1,n) > 0

KTT(m,n) = KHV(m,n+1) > 0 $\wedge$ KHU(m,n+2) > 0 $\wedge$ KHV(m+1,n+1) > 0

Hereafter, the arrays GEBVUY and GETVUY can be filled.

	KBB(m,n)	KB(m,n)	GEBVUY(m,n)	KT(m,n)	KTT(m,n)	GETVUY(m,n)
I	T	T	2	T	T	2
ii	T	T	2	T	F	1
iii	F	T	1	T	T	2
iv	F	T	1	T	F	1
v	T	T	2	F	F	0
vi	F	F	0	T	T	2
vii	F	T	1	F	F	0
viii	F	F	0	T	F	1
ix	other		0	other		0

Table II Definition of the arrays GEBVUY and GETVUY

The time dependent geometrical situation can now be distinguished and consequently the proper discretization in WAQUA (first/second order upwind or central or zero), [Stelling, 1984].

The boundary treatment of $S_y^c(u_{m,n})$ and $S_y^u(u''_{m,n})$ is as follows:

Determine the dry/wet status of the u velocity points by the arrays GEBVUY and GETVUY (Table II) at time t+½Δt.

$$S_y^c(u_{m,n}) \begin{cases} \dfrac{u_{m,n+2} + 4u_{m,n+1} - u_{m,n-2}}{12\Delta Y}, & \text{for situation (i)} \\ \dfrac{(u_{m,n+1} - u_{m,n-1})}{2\Delta Y}, & \text{for situation (ii) - (iv)} \\ 0, & \text{for situation (v) - (ix)} \end{cases} \quad (7.13)$$

The upwind difference operator depends on the flow pattern of the v velocity field.

If $\overline{\overline{v'}}_{m,n} > 0$:

$$S_y^u(u''_{m,n}) = \begin{cases} \dfrac{\left(3u''_{m,n} - 4u''_{m,n-1} + u''_{m,n-2}\right)}{2\Delta Y}, & \text{for situation GEBVUY = 2} \\ \dfrac{\left(u''_{m,n} - u''_{m,n-1}\right)}{\Delta Y}, & \text{for situation GEBVUY = 1} \\ 0, & \text{for situation GEBVUY = 0} \end{cases} \quad (7.14)$$

If $\overline{\overline{v'}}_{m,n} \leq 0$:

$$S_y^c(u''_{m,n}) = \begin{cases} \dfrac{\left(-3u''_{m,n} + 4u''_{m,n+1} - u''_{m,n+2}\right)}{2\Delta Y}, & \text{for situation GETVUY = 2} \\ \dfrac{\left(u''_{m,n+1} - u''_{m,n}\right)}{\Delta Y}, & \text{for situation GETVUY = 1} \\ 0, & \text{for situation GETVUY = 0} \end{cases} \quad (7.15)$$

Now we focus on another part of the righthand side of the adjoint v impulse equation associated with $\Delta V'_{m,n}$. Equation (3.102) originates from the discretization of the term uv_x at the second stage in the v impulse equation. The mathematical

derivation has been performed under the assumption that all surrounding points were always wet. Boundary effects and dryfall cause degenerations in the discretization of the term uv_x in WAQUA. In this case Table III has to be used. The necessary arrays GELUVX and GERUVX (Table VIII) have to be deduced from the WAQUA velocities at time $t+\Delta t$.

For example, if GELUVX(m-1,n) = 2 and GERUVX(m-1,n) = 1 follows from the flow field at time $t+\Delta t$ (situation (ii) in Table VIII) than the indicated degeneration takes place in equation (3.102). Situation (i) in Table III corresponds to the case were all surrounding points are wet.

	GELUVX, GERUVX		
	situation (i)	situation (ii)-(iv)	situation (v)-(ix)
v point m-2,n	$(\nu_v)''_{m-2,n}\left(\frac{\overline{\overline{u''}}_{m-2,n}}{12\Delta X}\right)$	X	X
v point m-1,n	$(\nu_v)''_{m-1,n}\left(\frac{4\overline{\overline{u''}}_{m-1,n}}{12\Delta X}\right)$	$(\nu_v)''_{m-1,n}\left(\frac{\overline{\overline{u''}}_{m-1,n}}{2\Delta X}\right)$	X
v point m+1,n	$-(\nu_v)''_{m+1,n}\left(\frac{4\overline{\overline{u''}}_{m+1,n}}{12\Delta X}\right)$	$-(\nu_v)''_{m+1,n}\left(\frac{\overline{\overline{u''}}_{m+1,n}}{2\Delta X}\right)$	X
v point m+2,n	$-(\nu_v)''_{m+2,n}\left(\frac{\overline{\overline{u''}}_{m+2,n}}{12\Delta X}\right)$	X	X

Table III The degenerations in equation (3.102)

A part of the righthand side of the adjoint v impulse equation consists of equation (3.105), a sort of adjoint upwind difference. Table IV shows the alterations in case of impeded geometry. Therefore, the arrays GERUVX and GELUVX (Table VIII) have to be calculated for the flow field at time t.

	GELUVX		
	2	1	0
v point m-2,n $\bar{\bar{u}}_{m-2,n} \le 0$	$(\nu_v)'_{m-2,n}\left(\frac{-\bar{\bar{u}}_{m-2,n}}{2\Delta X}\right)$	X	X
v point m-1,n $\bar{\bar{u}}_{m-1,n} \le 0$	$(\nu_v)'_{m-1,n}\left(\frac{4\bar{\bar{u}}_{m-1,n}}{2\Delta X}\right)$	$(\nu_v)'_{m-1,n}\left(\frac{\bar{\bar{u}}_{m-1,n}}{\Delta X}\right)$	X
v point m+1,n $\bar{\bar{u}}_{m,n} \le 0$	$(\nu_v)'_{m,n}\left(\frac{-3\bar{\bar{u}}_{m,n}}{2\Delta X}\right)$	$(\nu_v)'_{m,n}\left(\frac{-\bar{\bar{u}}_{m,n}}{\Delta X}\right)$	X

	GELUVX		
	2	1	0
v point m,n $\bar{\bar{u}}_{m,n} > 0$	$(\nu_v)'_{m,n}\left(\frac{3\bar{\bar{u}}_{m,n}}{2\Delta X}\right)$	$(\nu_v)'_{m,n}\left(\frac{\bar{\bar{u}}_{m,n}}{\Delta X}\right)$	X
v point m+1,n $\bar{\bar{u}}_{m+1,n} > 0$	$\left(\frac{-4\bar{\bar{u}}_{m+1,n}}{2\Delta X}\right)$	$(\nu_v)'_{m+1,n}\left(\frac{-\bar{\bar{u}}_{m+1,n}}{\Delta X}\right)$	X
v point m+2,n $\bar{\bar{u}}_{m+2,n} > 0$	$(\nu_v)'_{m+2,n}\left(\frac{\bar{\bar{u}}_{m+2,n}}{2\Delta X}\right)$	X	X

Table IV The degenerations in equation (3.105)

The terms corresponding to v point m,n contribute to the main diagonal. The other contribute to the righthand side (sign changes), due to the Jacobi method.

The last part left in these adjoint advective terms of this adjoint v impulse equation is equation (3.101). It consists of adjoint variables at the new time level, which set up the matrix structure, and adjoint variables at the old time level.

To determine the degenerations caused by impeded geometry an array GEOVVY has to be constructed from which the time-dependent local flow situation can be determined (Table V). In WAQUA impeded v velocity points which inhibit the flow of water are denoted by KHV ≤ 0.

KHV(m,n-1)	KHV(m,n)	KHV(m,n+1)	GEOVVY(m,n)
> 0	> 0	> 0	1: central
> 0	> 0	≤ 0	2: upwind
≤ 0	> 0	> 0	3: upwind
other			0: no advection

Table V Definition of array GEOVVY

The situation GEOVVY(m,n) = 1 corresponds to the case were the surrounding v points are wet. Now we focus on the other three situations. The coefficients $A_{m,n}$ and $C_{m,n}$ from the corresponding tridiagonal matrix equation can be read from Table VI. The array GEOVVY has to be constructed from the variables KHV at time t (Table V).

		GEOVVY		
		1	2	3
$A_{m,n}$	v point m,n-1	$\frac{v_{m,n}}{2\Delta Y}$	X	$\frac{v_{m,n-1}}{\Delta Y}$ if $v_{m,n-1} \leq 0$
$C_{m,n}$	v point m,+1	$-\frac{v_{m,n+1}}{2\Delta Y}$	$-\frac{v_{m,n+1}}{\Delta Y}$ if $v_{m,n+1} > 0$	X

Table VI The degenerations in equation (3.101)

For another contribution to the right side, the array GEOVVY has to be constructed from the variables KHV at time t+Δt (Table V).

	GEOVVY		
	1	2	3
v point m,n-1	$(\nu_v)''_{m,n-1}\left(\frac{v''_{m,n-1}}{2\Delta Y}\right)$	X	$(\nu_v)''_{m,n-1}\left(\frac{v''_{m,n-1}}{\Delta Y}\right)$ if $v'_{m,n-1} \leq 0$
v point m,+1	$(\nu_v)''_{m,n+1}\left(-\frac{v''_{m,n+1}}{2\Delta Y}\right)$	$(\nu_v)''_{m,n+1}\left(-\frac{v''_{m,n+1}}{\Delta Y}\right)$ if $v'_{m,n+1} > 0$	X

Table VII The degenerations in equation (3.101)

For convenience we give again the adjoint v impulse equation associated with $\Delta v'_{m,n}$, including the advective terms, neglecting the boundary treatment and the dryfall procedure (and the iterative aspect):

$$A_{m,n}\ \boxed{(\nu_v)'_{m,n-1}} + B_{m,n}\ \boxed{(\nu_v)'_{m,n}} + C_{m,n}\ \boxed{(\nu_v)'_{m,n+1}} = D_{m,n} \qquad (7.16)$$

with:

$$A_{m,n} = \frac{v_{m,n-1}}{2\Delta Y} \qquad (7.17)$$

$$B_{m,n} = \frac{2}{\Delta t} \qquad (7.18)$$

$$C_{m,n} = \frac{-v_{m,n+1}}{2\Delta Y} \qquad (7.19)$$

$$D_{m,n} = \frac{2}{\Delta t}(\nu_v)''_{m,n} + \overline{[f_{m,n} - fruv'_{m,n}]\left[(\nu_u)'_{m,n} + (\nu_u)''_{m,n}\right]}^{\xi\eta} \qquad (7.20)$$

$$- \frac{\left(v''_{m,n-1}(\nu_v)''_{m,n-1} - v''_{m,n+1}(\nu_v)''_{m,n+1}\right)}{2\Delta Y}$$

$$- (\nu_v)''_{m-2,n}\left(\frac{\overline{\overline{u''}}_{m-2,n}}{12\Delta X}\right) - (\nu_v)''_{m-1,n}\left(\frac{4\overline{\overline{u''}}_{m-1,n}}{12\Delta X}\right)$$

$$+ (\nu_v)''_{m+1,n}\left(\frac{4\overline{\overline{u''}}_{m+1,n}}{12\Delta X}\right) + (\nu_v)''_{m+2,n}\left(\frac{\overline{\overline{u''}}_{m+2,n}}{12\Delta X}\right)$$

$$- (\nu_u)''_{m,n}\tfrac{1}{4}S^u_y(u''_{m,n}) - (\nu_u)''_{m-1,n}\tfrac{1}{4}S^u_y(u''_{m-1,n})$$

$$- (\nu_u)''_{m-1,n+1}\tfrac{1}{4}S^u_y(u''_{m-1,n+1}) - (\nu_u)''_{m,n+1}\tfrac{1}{4}S^u_y(u''_{m,n+1})$$

$$- (\nu_u)'_{m,n}\tfrac{1}{4}S^c_y(u_{m,n}) - (\nu_u)'_{m-1,n}\tfrac{1}{4}S^c_y(u_{m-1,n})$$

$$- (\nu_u)'_{m-1,n+1}\tfrac{1}{4}S^c_y(u_{m-1,n+1}) - (\nu_u)'_{m,n+1}\tfrac{1}{4}S^c_y(u_{m,n+1})$$

Incorporating the boundary treatment and the dryfall procedure yields (still without the iterative aspect):

$$A_{m,n}\ \boxed{(\nu_v)'_{m,n-1}} + B_{m,n}\ \boxed{(\nu_v)'_{m,n}} + C_{m,n}\ \boxed{(\nu_v)'_{m,n+1}} = D_{m,n} \qquad (7.25)$$

- The coefficients $A_{m,n}$ and $C_{m,n}$ can be determined from Table VI
- One part of the righthand side $D_{m,n}$ is prescribed by Table VII. These elements have to be subtracted.
- The boundary treatment of the second operators S^c and S^u can be read from Table II. They appear in the formula for $D_{m,n}$.
- One part of the righthand side $D_{m,n}$ is prescribed by Table III. These elements have to be subtracted.

Now we deal with the iterative aspect, caused by the addition of equation (3.105).

Table IV shows the degenerations in case of impeded geometry. The arrays GERUVX and GELUVX (Table VIII) have to be calculated for the flow field at time t.

The elements corresponding to v point m,n contribute to the main diagonal of the tridiagonal matrix equation. The coefficients have to be added to $B_{m,n}$, dependent on the geometrical situation. The other elements in Table IV contain variables which are at right angles with the ones which set up a tridiagonal structure.

The iterative aspect: use values from the previous loop (at time $t+\Delta t$) in the first iteration. This way these elements have to be subtracted from the righthand side $D_{m,n}$. Applying the double sweep algorithm for solving the tridiagonal matrix equation yields a first guess for all adjoint v variables at time $t+½\Delta t$. The same strategy can be applied in the second iteration. All coefficients remain the same, except the other elements in Table IV. This first guess is used for the adjoint v variable at time $t+½\Delta t$. Applying the double sweep algorithm results in a second guess. It is expected that two iterations are enough for convergence.

•• Degenerations in the adjoint v impulse equation associated with $\Delta v_{m,n}$ caused by impeded geometry.

In procedure AD-SVU:

- Determine for all v velocity points the array GEOVVY (Table V) at time t.

$$(\nu_v)_{m,n} = DD_{m,n+1} - CC_{m,n+1}\left[(\nu_\zeta)_{m,n+1} - (\nu_\zeta)_{m,n} \right] \quad (7.26)$$

with:

$$CC_{m,n+1} = \frac{-(H^v)_{m,n}}{\Delta Y\left[\frac{2}{\Delta t} + frvv_{m,n} + AV \right]}$$

$$DD_{m,n+1} = \frac{\left[\frac{2}{\Delta t} - frvv_{m,n} - AVD \right](\nu_v)'_{m,n}}{\left[\frac{2}{\Delta t} + frvv_{m,n} + AV \right]}$$

$$- \frac{(H^v)_{m,n}\left[(\nu_\zeta)'_{m,n} - (\nu_\zeta)'_{m,n+1} \right]}{\Delta Y\left[\frac{2}{\Delta t} + frvv_{m,n} + AV \right]}$$

- If GEOVVY(m,n) = 1:

$$AV = \frac{\left(\bar{v}'_{m,n+1} - \bar{v}'_{m,n-1} \right)}{2\Delta Y} \quad (7.27)$$

$$AVD = \frac{\left(v'_{m,n+1} - v'_{m,n-1} \right)}{2\Delta Y}$$

- If GEOVVY(m,n) = 2:

$$AV = \frac{\left(\bar{v}'_{m,n} - \bar{v}'_{m,n-1} \right)}{\Delta Y}, \text{ if } \bar{v}'_{m,n} > 0 \quad (7.28)$$

$$= 0, \quad \text{otherwise}$$

$$AVD = \frac{\left(v'_{m,n} - v'_{m,n-1} \right)}{\Delta Y}, \text{ if } v_{m,n} > 0$$

$$= 0, \quad \text{otherwise}$$

- If GEOVVY(m,n) = 3:

$$AV = \frac{\left(v'_{m,n+1} - v'_{m,n} \right)}{\Delta Y}, \text{ if } v'_{m,n} \le 0 \qquad (7.29)$$

$$= 0, \quad \text{otherwise}$$

$$AVD = \frac{\left(v'_{m,n+1} - v'_{m,n} \right)}{\Delta Y}, \text{ if } v_{m,n} \le 0$$

$$= 0, \quad \text{otherwise}$$

So far, we handled the degenerations in the adjoint advective terms caused by impeded points in the adjoint v impulse equation.

•• Degenerations in the adjoint u impulse equation associated with $\Delta u_{m,n}$ caused by impeded geometry.

In the adjoint u impulse equation associated with $\Delta u_{m,n}$ the second order difference operators S^c (central) and S^u (upwind) appear. Here the boundary treatment of these operators in the adjoint computation process is indicated. These approximations depend on the dry/wet status of the surrounding points. Therefore, the (time-dependent) local flow situation has to be determined first to figure out which approximation has been used in the computation process of WAQUA.

- $S^c_x(v'_{m,n})$ and $S^u_x(v'_{m,n})$ in (3.109) and (3.110)

We define for each v velocity point the logical arrays KLL, KL, KR and KRR with which the arrays GELUVX and GERUVX are determined.

KLL(m,n) = KHU(m-2,n)> 0 $\wedge$ KHV(m-2,n) > 0 $\wedge$ KHU(m-2,n+1) > 0

KL(m,n) = KHU(m-1,n)> 0 $\wedge$ KHV(m-1,n) > 0 $\wedge$ KHU(m-1,n+1) > 0

KR(m,n) = KHU(m,n) > 0 $\wedge$ KHV(m+1,n) > 0 $\wedge$ KHU(m,n+1) > 0

KRR(m,n) = KHU(m+1,n) > 0 $\wedge$ KHV(m+2,n) > 0 $\wedge$ KHU(m+1,n+1) > 0

Hereafter, the arrays GELUVX and GERUVX can be filled.

	KLL(m,n)	KL(m,n)	GELUVX (m,n)	KR(m,n)	KRR(m,n)	GERUVX (m,n)
I	T	T	2	T	T	2
ii	T	T	2	T	F	1
iii	F	T	1	T	T	2
iv	F	T	1	T	F	1
v	T	T	2	F	F	0
vi	F	F	0	T	T	2
vii	F	T	1	F	F	0
viii	F	F	0	T	F	1
ix	other		0	other		0

Table VIII Definition of the arrays GELUVX and GERUVX

With this information the local flow situation can be determined and consequently which approximation for the v_x term has been used in WAQUA (first/second order upwind or central or zero), [Stelling, 1984]. This is necessary for the proper form of the adjoint advective terms in the adjoint computation process.

The boundary treatment of $S_x^c(\bar{v}'_{m,n})$ and $S_x^u(v'_{m,n})$ is as follows:

- Determine the dry/wet status of the v velocity points by the arrays GELUVX and GERUVX (Table VIII) at time t.

$$S_x^c(\bar{v}'_{m,n}) = \begin{cases} \dfrac{\left[\bar{v}'_{m+2,n} + 4\bar{v}'_{m+1,n} - 4\bar{v}'_{m-1,n} - \bar{v}'_{m-2,n}\right]}{12\Delta X} & \text{, for situation (i)} \\ \dfrac{\left(\bar{v}'_{m+1,n} - \bar{v}'_{m-1,n}\right)}{2\Delta X} & \text{, for situation (ii)} - \text{(iv)} \\ 0 & \text{, for situation (v)} - \text{(ix)} \end{cases} \tag{7.30}$$

The upwind difference operator depends on the flow pattern of the u velocity field.

If $\bar{\bar{u}}_{m,n} > 0$:

$$S_x^u(v'_{m,n}) = \begin{cases} \dfrac{\left(3v'_{m,n} - 4v'_{m-1,n} + v'_{m-2,n}\right)}{2\Delta X} & \text{, for situation GELUVX= 2} \\ \dfrac{\left(v'_{m,n} - v'_{m-1,n}\right)}{\Delta X} & \text{, for situation GELUVX= 1} \\ 0 & \text{, for situation GELUVX= 0} \end{cases} \tag{7.31}$$

If $\bar{\bar{u}}_{m,n} \leq 0$:

$$S_x^u(v'_{m,n}) = \begin{cases} \dfrac{\left(-3v'_{m,n} + 4v'_{m-1,n} - v'_{m+2,n}\right)}{2\Delta X} & \text{, for situation GERUVX= 2} \\ \dfrac{\left(v'_{m,n} - v'_{m,n}\right)}{\Delta X} & \text{, for situation GERUVX= 1} \\ 0 & \text{, for situation GERUVX= 0} \end{cases} \quad (7.32)$$

Another part of the righthand side of the adjoint u impulse equation under consideration forms equation (3.108). Table IX shows the degenerations in case of impeded geometry.

The necessary arrays GEBVUY and GETVUY (Table II) have to be deduced from the flow field at time t+½Δt.

	GEBVUY, GETVUY		
	situation (i)	situation (ii)-(iv)	situation (v)-(ix)
u point m,n+2	$-(\nu_u)'_{m,n-2}\left(\dfrac{\bar{\bar{v}}'_{m,n+2}}{12\Delta Y}\right)$	X	X
u point m,n+1	$-(\nu_u)'_{m,n+1}\left(\dfrac{4\bar{\bar{v}}'_{m,n+1}}{12\Delta Y}\right)$	$-(\nu_u)'_{m,n+1}\left(\dfrac{\bar{\bar{v}}'_{m,n+1}}{2\Delta Y}\right)$	X
u point m,n-1	$(\nu_u)'_{m,n-1}\left(\dfrac{4\bar{\bar{v}}'_{m,n-1}}{12\Delta Y}\right)$	$(\nu_u)'_{m,n-1}\left(\dfrac{\bar{\bar{v}}'_{m,n-1}}{2\Delta Y}\right)$	X
u point m,n-2	$(\nu_u)''_{m,n-2}\left(\dfrac{\bar{\bar{v}}'_{m,n-2}}{12\Delta Y}\right)$	X	X

Table IX The degenerations in equation (3.108)

Then, the part of the right side originating from the second order upwind difference in WAQUA. Table X shows the deformations caused by impeded geometry. The arrays GEBVUY and GETVUY (Table II) have to be deduced from the flow situation at time t-½Δt.

	GEBVUY		
	2	1	0
u point m,n+2 $\overset{='}{v}_{m,n+2} > 0$	$(\nu_u)_{m,n+2}\left(\frac{+\overset{='}{v}_{m,n+2}}{2\Delta Y}\right)$	X	X
u point m,n+1 $\overset{='}{v}_{m,n+1} > 0$	$(\nu_u)_{m,n+1}\left(\frac{-4\overset{='}{v}_{m,n+1}}{2\Delta Y}\right)$	$(\nu_u)_{m,n+1}\left(\frac{\overset{='}{v}_{m,n+1}}{\Delta Y}\right)$	X
u point m,n $\overset{='}{v}_{m,n} > 0$	$(\nu_u)_{m,n}\left(\frac{3\overset{='}{v}_{m,n}}{2\Delta Y}\right)$	$(\nu_u)_{m,n}\left(\frac{\overset{='}{v}_{m,n}}{\Delta Y}\right)$	X

	GETVUY		
	2	1	0
u point m,n $\overset{='}{v}_{m,n} \le 0$	$(\nu_u)_{m,n}\left(\frac{-3\overset{='}{v}_{m,n}}{2\Delta Y}\right)$	$(\nu_u)_{m,n}\left(\frac{\overset{='}{v}_{m,n}}{\Delta Y}\right)$	X
u point m,n-1 $\overset{='}{v}_{m,n-1} \le 0$	$(\nu_u)_{m,n-1}\left(\frac{4\overset{='}{v}_{m,n-1}}{2\Delta Y}\right)$	$(\nu_u)_{m,n-1}\left(\frac{\overset{='}{v}_{m,n-1}}{\Delta Y}\right)$	X
u point m,n-2 $\overset{='}{v}_{m,n-2} \le 0$	$(\nu_u)_{m,n-2}\left(\frac{-\overset{='}{v}_{m,n-2}}{2\Delta Y}\right)$	X	X

Table X The degenerations in equation (3.108)

The elements corresponding to u point m,n contribute to the main diagonal of the matrix equation. The coefficients have to be added to $B_{m,n}$. The other elements influence the right side, since an iterative solution method is proposed.

To determine the deformations caused by impeded geometry for equation (3.107) an array GEOUUX has to be determined (Table I) from the variables KHU at time t-½Δt. The coefficients $A_{m,n}$ and $C_{m,n}$ from the corresponding tridiagonal matrix equation can be read from Table XI.

		GEOUUX		
		1	2	3
$A_{m,n}$	u point m-1,n	$\frac{u'_{m-1,n}}{2\Delta X}$	X	$\frac{u'_{m-1,n}}{\Delta X}$ if $u'_{m-1,n} \le 0$
$C_{m,n}$	u point m+1,n	$-\frac{u'_{m+1,n}}{2\Delta X}$	$-\frac{u'_{m+1,n}}{\Delta X}$ if $u'_{m+1,n} > 0$	X

Table XI The degenerations in equation (3.107)

For another contribution to the right side, the array GEOUUX has to be constructed from the variables KHU at time t+½Δt (Table I).

	GEOUUX		
	1	2	3
u point m-1,n	$(\nu_u)'_{m-1,n}\left(\frac{u'_{m-1,n}}{2\Delta X}\right)$	X	$(\nu_u)'_{m-1,n}\left(\frac{u'_{m-1,n}}{\Delta X}\right)$ if $u_{m-1,n} \le 0$
u point m+1,n	$(\nu_u)'_{m+1,n}\left(-\frac{u'_{m+1,n}}{2\Delta X}\right)$	$(\nu_u)'_{m+1,n}\left(-\frac{u'_{m+1,n}}{\Delta X}\right)$ if $u_{m+1,n} > 0$	X

Table XII The degenerations in equation (3.107)

For convenience we give again the adjoint u impulse equation associated with $\Delta u_{m,n}$, including the advective terms, neglecting the boundary treatment and the dryfall procedure (and the iterative aspect):

$$A_{m,n}\ [(\nu_u)_{m-1,n}] + B_{m,n}\ [(\nu_u)_{m,n}] + C_{m,n}\ [(\nu_u)_{m+1,n}] = D_{m,n} \qquad (7.33)$$

with:

$$A_{m,n} = \frac{\bar{u}'_{m-1,n}}{2\Delta X} \qquad (7.34)$$

$$B_{m,n} = \frac{2}{\Delta t} \qquad (7.35)$$

$$C_{m,n} = \frac{-\bar{u}'_{m+1,n}}{2\Delta X} \qquad (7.36)$$

$$D_{m,n} = \frac{2}{\Delta t}(\nu_u)'_{m,n} - \overline{[f_{m,n} - frvu_{m,n}]\ [(\nu_v)_{m,n} + (\nu_v)'_{m,n}]}^{\eta\xi} \qquad (7.37)$$

$$- \frac{\left(u'_{m-1,n}(\nu_u)_{m-1,n} - u'_{m+1,n}(\nu_u)'_{m+1,n} \right)}{2\Delta X} \qquad (7.38)$$

$$- (\nu_u)'_{m,n-2}\left(\frac{\overline{\overline{v'}}_{m,n-2}}{12\Delta Y}\right) - (\nu_u)'_{m,n-1}\left(\frac{4\overline{\overline{v'}}_{m,n-1}}{12\Delta Y}\right)$$

$$+ (\nu_u)'_{m,n+1}\left(\frac{4\overline{\overline{v'}}_{m,n+1}}{12\Delta Y}\right) + (\nu_u)'_{m,n+2}\left(\frac{\overline{\overline{v'}}_{m,n+2}}{12\Delta Y}\right) \qquad (7.39)$$

$$- (\nu_v)'_{m,n}\tfrac{1}{4}S^u_x(v'_{m,n}) - (\nu_v)'_{m+1,n}\tfrac{1}{4}S^u_x(v'_{m+1,n}) \qquad (7.40)$$

$$- (\nu_v)'_{m+1,n-1}\tfrac{1}{4}S^u_x(v'_{m+1,n-1}) - (\nu_v)'_{m,n-1}\tfrac{1}{4}S^u_x(v'_{m,n-1})$$

$$- (\nu_v)_{m,n}\tfrac{1}{4}S^c_x(\bar{v}'_{m,n}) - (\nu_v)_{m+1,n}\tfrac{1}{4}S^c_x(\bar{v}'_{m+1,n}) \qquad (7.41)$$

$$- (\nu_v)_{m+1,n-1}\tfrac{1}{4}S^c_x(\bar{v}'_{m+1,n-1}) - (\nu_v)_{m,n-1}\tfrac{1}{4}S^c_x(\bar{v}'_{m,n-1})$$

- The coefficients $A_{m,n}$ and $C_{m,n}$ can be determined from Table XI.

- One part of the righthand side $D_{m,n}$ is prescribed by Table XII. These elements have to be subtracted.

- The boundary treatment of the second operators S^c and S^u can be read from Table VIII. They appear in the formula for $D_{m,n}$.

- One part of the righthand side $D_{m,n}$ is prescribed by Table IX. These elements have to be subtracted.

- Now we deal with the iterative aspect, caused by the addition of equation (3.111).

Table X shows the degenerations in case of impeded geometry. The arrays GEBVUY and GETVUY (Table VIII) have to be calculated for the flow field at time t.

The elements corresponding to u point m,n contribute to the main diagonal of the tridiagonal matrix equation. The coefficients have to be added to $B_{m,n}$, dependent on the geometrical situation. The other elements in Table X contain variables which are at right angles with the ones which set up a tridiagonal structure.

The iterative aspect: use values from the previous loop (at time $t+\frac{1}{2}\Delta t$) in the first iteration. This way these elements have to be subtracted from the righthand side $D_{m,n}$. Applying the double sweep algorithm for solving the tridiagonal matrix equation yields a first guess for all adjoint u variables at time t. The same strategy can be applied in the second iteration. All coefficients remain the same, except the other elements in Table X. This first guess is used for the adjoint u variable at time t. Applying the double sweep algorithm results in a second guess. It is expected that two iterations are enough for convergence.

7.4.2. Open Boundaries

Open boundaries are introduced to restrict the size of the domain of the problem. The numerical boundary procedures for an open water level boundary are described by [Stelling, 1984]. The solution at the inner points is not greatly influenced by the order of the advection discretization near the open boundary, [Stelling, 1984]. At inflow uu_x is approximated by a zero value, otherwise first order upwind. The influence on the inner points of this approximation is negligible as was found by practical experiments, [Stelling, 1984]. Therefore, it is

proposed to neglect the boundary treatment of the terms uu_x (and vv_y) in the adjoint computation process.

Example: if m,n is a left water level boundary point, then GEOUUX(m,n) and GEOUUX(m+1,n) equal zero. The treatment of GEOVVY near a water level boundary is similar.

7.4.3. Spherical and curvilinear coordinates

The boundary treatment and the degenerations caused by impeded points is similar to the case for rectangular WAQUA. For curvilinear models they are:

- In all equations: ΔX must be replaced by $\Delta\xi$ and ΔY by $\Delta\eta$.
- The variables AU1 and AU1D have to be multiplied by $\frac{1}{K^u_{m,n}}$ in (7.9)
- The definition of the second operators has to be used ((3.114) ··· (3.117))
- In Table III and Table IV the adjoint v velocity has to be multiplied by the corresponding $\frac{1}{K}$
- In Table VI and Table VII the v velocity has to be multiplied by the corresponding $\frac{1}{E^v}$
- The variables AV and AVD has to be multiplied by $\frac{1}{E^v_{m,n}}$ in (7.26)
- In Table IX and Table X the adjoint u velocity has to be multiplied by the corresponding $\frac{1}{E}$
- In Table XI and Table XII the u velocity has to be multiplied by the corresponding $\frac{1}{K^u}$